

10/513699

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introduction of free HIT display format
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NEWS 15 MAY 28 CAS databases on STN enhanced with NANO super role in
records back to 1992
NEWS 16 JUN 01 CAS REGISTRY Source of Registration (SR) searching
enhanced on STN
NEWS 17 JUN 26 NUTRACEUT and PHARMAML no longer updated
NEWS 18 JUN 29 IMSCOPROFILE now reloaded monthly
NEWS 19 JUN 29 EPFULL adds SLART to AB, MCLM, and TI fields
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<12/04/2007>

Erich Leese

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FILE 'HOME' ENTERED AT 18:23:43 ON 29 JUN 2009

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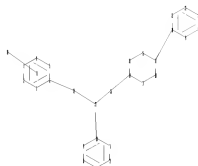
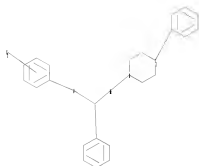
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<http://www.cas.org/support/stngen/stdoc/properties.html>

=>

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chain nodes :
25 26 27 30
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24
chain bonds :
6-25 10-27 14-26 17-20 25-27 26-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24
exact/norm bonds :
6-25 10-27 13-14 13-18 14-15 14-26 15-16 16-17 17-18 17-20 25-27 26-27
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24
20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

```

G1:C,N

G2:CF2,CF3,CC12,CC13,CBr2,CBr3,X

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G3:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 30:CLASS
31:Atom

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

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Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

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FULL SEARCH INITIATED 18:24:31 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 20268 TO ITERATE

100.0% PROCESSED 20268 ITERATIONS

211 ANSWERS

SEARCH TIME: 00.00.02

L2 211 SEA SSS FUL L1

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COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

185.88 186.10

FILE 'CAPLUS' ENTERED AT 18:24:36 ON 29 JUN 2009

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FILE COVERS 1907 - 29 Jun 2009 VOL 151 ISS 1

FILE LAST UPDATED: 28 Jun 2009 (20090628/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009

<12/04/2007>

Erich Leese

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USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2009

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 12 full

L3 17 L2

=> d ibib abs hitstr tot

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DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L3 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:412461 CAPLUS

DOCUMENT NUMBER: 151:496

TITLE: QSAR study of the 5-HT1A receptor affinities of arylpiperazines using a genetic algorithm-artificial neural network model

AUTHOR(S): Habibi-Yangjeh, Aziz

CORPORATE SOURCE: Department of Chemistry, Faculty of Science, University of Mohaghegh Ardabili, Ardabil, Iran
Monatshefte fuer Chemie (2009), 140(5), 523-530
CODEN: MOCMB7; ISSN: 0026-9247

PUBLISHER: SpringerWienNewYork

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Genetic algorithm-multiparameter linear regression (GA-MLR) and genetic algorithm-artificial neural network (GA-ANN) models have been used for prediction of the 5-HT1A receptor affinities (pK i) of 66 arylpiperazines. A large number of theor. descriptors were calculated for each compound The genetic

algorithm (GA) was used for selection of the variables that resulted in the best fit to the MLR and ANN models. The models were generated using seven descriptors as variables. For evaluation of the predictive power of the models, pK i values of 13 compds. in the prediction set were calculated. Mean percentage deviation (MPD) for the GA-MLR and GA-ANN models were 0.344 and 0.065, resp. Comparison of the results obtained by use of the models reveals the GA-ANN model is superior to the GA-MLR model.
Graphical abstract

IT 328248-21-1 328248-24-4 328248-30-2

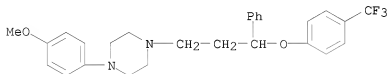
328248-36-8 753439-74-6 767277-20-3
777843-82-0

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(QSAR study of 5-HT1A receptor affinities of arylpiperazines using a genetic algorithm-artificial neural network model)

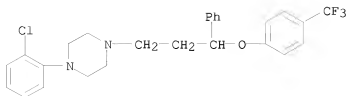
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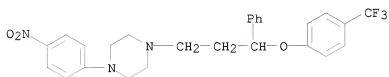
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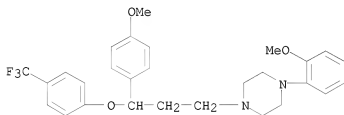
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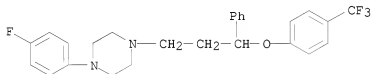
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CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 753439-74-6 CAPLUS

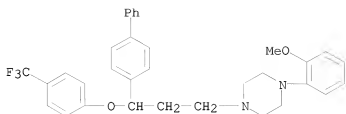
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RN 767277-20-3 CAPLUS

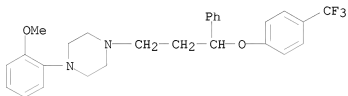
CN Piperazine, 1-[3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)

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RN 777843-82-0 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



REFERENCE COUNT:

46

THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:986436 CAPLUS

DOCUMENT NUMBER: 150:321888

TITLE: The structure-based 3D-QSAR study of MCH1 receptor antagonists

AUTHOR(S): Lee, New Gil; Yoo, Seung-Eun; Kang, Nam Sook

CORPORATE SOURCE: Korea Research Institute of Chemical Technology, Daejeon, S. Korea

SOURCE: Molecular Simulation (2008), 34(7), 699-705

CODEN: MOSIEA; ISSN: 0892-7022

PUBLISHER: Taylor & Francis Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Melanin-concentrating hormone 1 receptor (MCH1-R) mediates the orexigenic effects

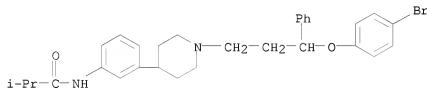
of melanin-concentrating hormone and its antagonist, are considered as a potential targets for the treatment of obesity. To design more potent and selective MCH1-R antagonists, at first, the authors built up the homol. structure of MCH1-R. Then, the authors carried out the receptor based 3 dimensional Quant. Structure Activity Relationship (3D-QSAR) using comparative mol. field anal. and Comparative Mol. Similarity Indexes Anal. (CoMSIA) for a series of scaffold of MCH1-R antagonists and the docking study for MCH1-R. These models are proved as statistically valid models with a good correlative and predictive power. Based on these models, the authors are going to develop more potent and selective MCH1-R antagonists.

IT 1132777-99-1

RL: PEP (Physical, engineering or chemical process); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses) (structure-based 3D-QSAR study of MCH1 receptor antagonists as anti-obesity drugs)

RN 1132777-99-1 CAPLUS

CN Propanamide, N-[3-[1-[3-(4-bromophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2008:803320 CAPLUS

DOCUMENT NUMBER: 149:215113

TITLE: Two-dimensional QSAR studies on arylpiperazines as high-affinity 5-HT1A receptor ligands

AUTHOR(S): Weber, Karen C.; Honorio, Kathia M.; Andricopulo, Adriano D.; Da Silva, Alberico B. F.

CORPORATE SOURCE: Instituto de Quimica de Sao Carlos, Universidade de

Sao Paulo, Sao Carlos, 13560-970, Brazil

SOURCE: Medicinal Chemistry (2008), 4(4), 328-335

CODEN: MCEHAJ; ISSN: 1573-4064

PUBLISHER: Bentham Science Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 5-HT1A receptor plays an important role in the delayed onset of antidepressant action of a class of selective serotonin reuptake inhibitors. Moreover, 5-HT1A receptor levels have been shown to be altered in patients suffering from major depression. In this work, hologram quant. structure-activity relationship (HQ SAR) studies were performed on a series of arylpiperazine compds. presenting affinity to the 5-HT1A receptor. The models were constructed with a training set of 70 compds. The most significant HQ SAR model ($q^2 = 0.81$, $r^2 = 0.96$) was generated using atoms, bonds, connections, chirality, and donor and acceptor as fragment distinction, with fragment size of 6-9. Predictions for an external test set containing 20 compds. are in good agreement with exptl. results showing the robustness of the model. Addnl., useful information can be obtained from the 2D contribution maps.

IT 328248-15-3 328248-21-1 328248-24-4

328248-30-2 328248-36-8 753439-74-6

767277-20-3 777843-82-0

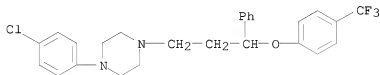
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(two-dimensional QSAR studies on arylpiperazines as high-affinity 5-HT1A receptor ligands)

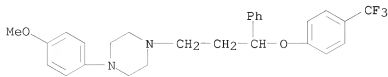
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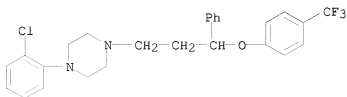
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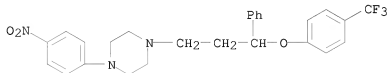
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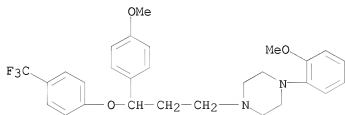
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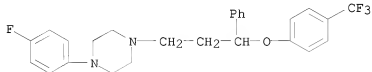
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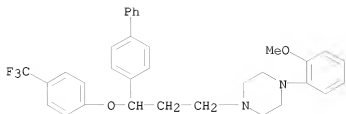
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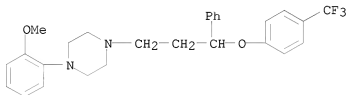
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10/513699



RN 777843-82-0 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



REFERENCE COUNT:

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THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:767635 CAPLUS

DOCUMENT NUMBER: 149:324283

TITLE: Quantitative structure-affinity relationship of 5-HT1A receptor ligands by the classification tree method

AUTHOR(S): Kuz'min, V. E.; Polischuk, P. G.; Artemenko, A. G.; Makan, S. Yu.; Andronati, S. A.

CORPORATE SOURCE: A.V. Bogatsky Physical-Chemical Institute, National Academy of Sciences of Ukraine, Odessa, Ukraine
SOURCE: SAR and QSAR in Environmental Research (2008), 19(3-4), 213-244

CODEN: SQERED; ISSN: 1062-936X

PUBLISHER: Taylor & Francis Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The influence of mol. structure of 346 ligands on their affinity for 5-HT1A receptors was investigated. It was shown that the effectiveness of the proposed novel approach for interpretation of decision tree models compared favorably with the PLS method. In the context of the proposed approach, mol. fragments and their values of the relative influence on the affinity for 5-HT1A receptors were defined.

IT 328248-15-3 328248-21-1 328248-24-4

328248-30-2 328248-36-8 753439-74-6

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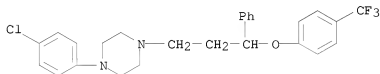
RL: ANT (Analyte); BSU (Biological study, unclassified); PRP (Properties);

ANST (Analytical study); BIOL (Biological study)

(quant. structure-affinity relationship of 5-HT1A receptor ligands by the classification tree method)

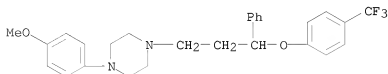
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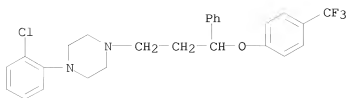
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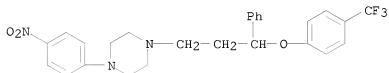
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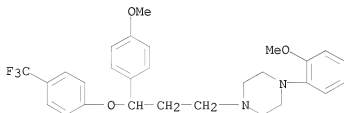
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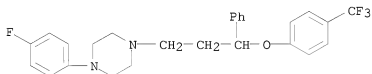
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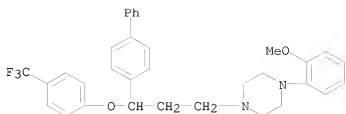
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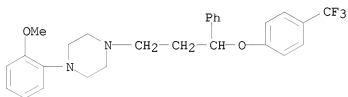
CN Piperazine, 1-[3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)

10/513699



RN 777843-82-0 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



REFERENCE COUNT:

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THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:232006 CAPLUS

DOCUMENT NUMBER: 148:440268

TITLE: A chemometric study of the 5-HT1A receptor affinities presented by arylpiperazine compounds

AUTHOR(S): Weber, Karen C.; da Silva, Alberico B. F.

CORPORATE SOURCE: Instituto de Química de São Carlos, Universidade de São Paulo, São Carlos, 13566-590, Brazil

SOURCE: European Journal of Medicinal Chemistry (2008), 43(2), 364-372

CODEN: EJMCA5; ISSN: 0223-5234

PUBLISHER: Elsevier Masson SAS

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Arylpiperazine compds. are promising 5-HT1A receptor ligands that can contribute for accelerating the onset of therapeutic effect of selective serotonin reuptake inhibitors. In the present work, the chemometric methods HCA, PCA, KNN, SIMCA and PLS were employed in order to obtain SAR and QSAR models relating the structures of arylpiperazine compds. to their 5-HT1A receptor affinities. A training set of 52 compds. was used to construct the models and the best ones were obtained with nine topol. descriptors. The classification and regression models were externally validated by means of predictions for a test set of 14 compds. and have presented good quality, as verified by the correctness of classifications, in the case of pattern recognition studies, and by the high correlation coeffs. ($q^2 = 0.76$, $r^2 = 0.83$) and small prediction errors for the PLS regression. Since the results are in good agreement with previous SAR studies, we can suggest that these findings can help in the search for 5-HT1A receptor ligands that are able to improve antidepressant treatment.

IT 328248-21-1 328248-24-4 328248-30-2

328248-36-8 753439-74-6 767277-20-3

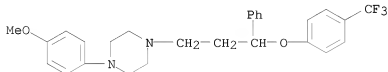
777843-82-0

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(chemometric study of 5-HT1A receptor affinities presented by arylpiperazine compds. as possible antidepressants)

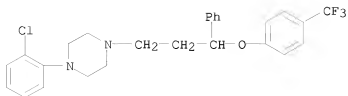
RN 328248-21-1 CAPLUS

CN Piperazine, 1-(4-methoxyphenyl)-4-[3-phenyl-3-(4-(trifluoromethyl)phenoxy)propyl]- (CA INDEX NAME)



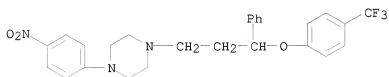
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CN Piperazine, 1-(2-chlorophenyl)-4-[3-phenyl-3-(4-(trifluoromethyl)phenoxy)propyl]- (CA INDEX NAME)



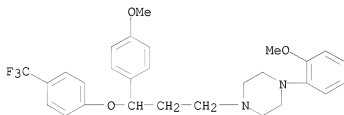
RN 328248-30-2 CAPLUS

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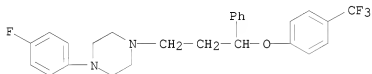
RN 328248-36-8 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 753439-74-6 CAPLUS

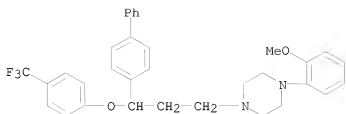
CN Piperazine, 1-(4-fluorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 767277-20-3 CAPLUS

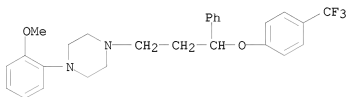
CN Piperazine, 1-[3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)

10/513699



RN 777843-82-0 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-(4-(trifluoromethyl)phenoxy)propyl]- (CA INDEX NAME)

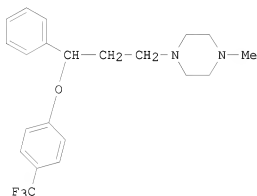


REFERENCE COUNT:

35

THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2006:847178 CAPLUS
 DOCUMENT NUMBER: 145:410017
 TITLE: Synthesis of benzenepropanamine analogues as non-detergent spermicides with antitrichomonas and anticandida activities
 AUTHOR(S): Kumar, S. T. V. S. Kiran; Sharma, Vishnu Lal; Kumar, Manish; Shukla, Praveen Kumar; Tiwari, Pratibha; Jain, Rajeev Kumar; Maikhuri, Jagdamba Prasad; Singh, Divya; Gupta, Gopal; Singh, Man Mohan
 CORPORATE SOURCE: Division of Medicinal and Process Chemistry, Central Drug Research Institute, Lucknow, 226001, India
 SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(19), 6593-6600
 CODEN: BMECEP; ISSN: 0968-0896
 PUBLISHER: Elsevier Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 145:410017
 GI



I

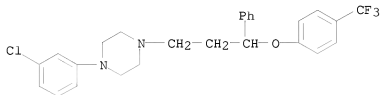
- AB Fifteen analogs of benzenepropanamine were synthesized and evaluated for their spermicidal as well as microbicidal activities against *Trichomonas vaginalis* and *Candida* spp. Several compds. showed appreciable dual activities. Compound I exhibited good spermicidal (MEC = 0.1%) along with substantial anticandidal (MIC = 0.05%) activities, while compds. 3 and 6 showed significant microbicidal activities with moderate spermicidal effect. The SAR of these structures is being discussed here in this communication. It is concluded that suitable structural modifications in this class of compds. at 3-amino position may lead to a potent spermicide with associated microbicidal activity.
- IT 911811-08-0P 911811-09-1P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

10/513699

(benzenepropanamine analogs as non-detergent spermicides with antitrichomonas and anticandida activities)

RN 911811-08-0 CAPLUS

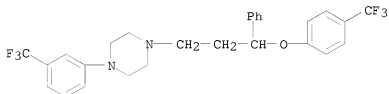
CN Piperazine, 1-(3-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 911811-09-1 CAPLUS

CN Piperazine, 1-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1143268 CAPLUS

DOCUMENT NUMBER: 144:63874

TITLE: Design and synthesis of long-chain arylpiperazines with mixed affinity for serotonin transporter (SERT) and 5-HT1A receptor

AUTHOR(S): Perrone, Roberto; Berardi, Francesco; Colabufo, Nicola A.; Lacivita, Enza; Larizza, Carmela; Leopoldo, Marcello; Tortorella, Vincenzo

CORPORATE SOURCE: Dipartimento Farmaco-Chimico, Universita degli Studi di Bari, Bari, 70125, Italy

SOURCE: Journal of Pharmacy and Pharmacology (2005), 57(10), 1319-1327

CODEN: JPPMAB; ISSN: 0022-3573

PUBLISHER: Pharmaceutical Press

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:63874

AB A new generation of antidepressant agents could be represented by compds. with mixed activity as serotonin transporter (SERT) inhibitors and 5-HT1A receptor antagonists. We report here on the synthesis and evaluation of SERT and 5-HT1A receptor affinity of long-chain arylpiperazines obtained either by modifying 6-nitroquipazine into a long-chain arylpiperazine or by inserting a modified 6-nitroquipazine moiety or other structures endowed with SERT affinity into a long-chain arylpiperazine with 5-HT1A affinity. Among the compds. studied, 2-[4-(2-methoxyphenyl)piperazin-1-yl]-N-(6-nitro-2-quinolyl)ethylamine (21) and 1-(5-bromo-1,2,3,4-tetrahydronaphthalen-1-yl)-3-[4-(2-methoxyphenyl)-piperazin-1-yl]-1-propanone (24) showed good affinity values for SERT and 5-HT1A receptors (SERT: Ki (inhibition constant) = 71.8 and 62.8 nM; 5-HT1A Ki = 14.2 and 0.82 nM, resp.).

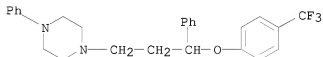
IT 871739-17-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(aryl)piperazines with mixed affinity for serotonin transporter and 5-HT1A receptor)

RN 871739-17-2 CAPLUS

CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:2) (CA INDEX NAME)



●2 HCl

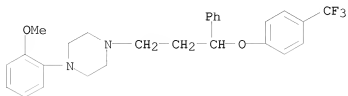
IT 777843-82-0

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(aryl)piperazines with mixed affinity for serotonin transporter and

10/513699

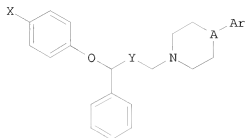
5-HT1A receptor)
RN 777843-82-0 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-(4-(trifluoromethyl)phenoxy)propyl]- (CA INDEX NAME)



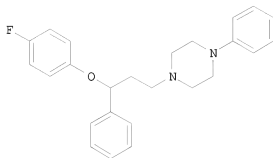
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2005:1103625 CAPLUS
 DOCUMENT NUMBER: 143:387060
 TITLE: Preparation of piperazine or piperidine derivatives as
 serotonin reuptake inhibitors
 INVENTOR(S): Pinney, Kevin G.; Miranda, Maria Graciela; Dorsey,
 James Michael
 PATENT ASSIGNEE(S): Baylor University, USA
 SOURCE: PCT Int. Appl., 52 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|-----------------|------------|
| WO 2005094896 | A2 | 20051013 | WO 2005-US10356 | 20050328 |
| WO 2005094896 | A3 | 20070503 | | |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | |
| RW: | BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AP, EA, EP, OA | | | |
| EP 1732610 | A2 | 20061220 | EP 2005-730778 | 20050328 |
| R: | AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU | | | |
| US 20080132514 | A1 | 20080605 | US 2007-594105 | 20070921 |
| PRIORITY APPLN. INFO.: | | | US 2004-557069P | P 20040326 |
| | | | WO 2005-US10356 | W 20050328 |
| OTHER SOURCE(S): | CASREACT 143:387060; MARPAT 143:387060 | | | |
| GI | | | | |



I



II

AB Title compds. I [X = F or CF₃; Y = (CH₂)_n; n = 0-1; A = N or C; Ar = aryl] and their pharmaceutically acceptable salts, are prepared and disclosed as serotonin reuptake inhibitors. Thus, e.g., II was prepared by reduction of 1-phenyl-3-(4-phenyl-piperazin-1-yl)-propan-1-ol (preparation given) using sodium borohydride followed by coupling with 4-fluorophenol. The ability of I to inhibit [3H]5-HT uptake was evaluated using liquid scintillation spectroscopy and it was revealed that selected compds. of the invention possessed IC₅₀ values in the range of 1.45 up to 9.56 μM. I as serotonin reuptake inhibitors should prove useful in the treatment of depression. Pharmaceutical composition comprising I are disclosed.

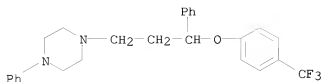
IT 158545-85-8P 691872-56-7P 691872-58-9P
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 691872-66-9P 866548-21-2P 866548-22-3P
 866548-23-4P 866548-24-5P 866548-25-6P
 866548-26-7P 866548-27-8P 866548-28-9P
 866548-29-0P 866548-30-3P 866548-31-4P
 866548-36-9P 866548-37-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of piperazine or piperidine derivs. as serotonin reuptake inhibitors)

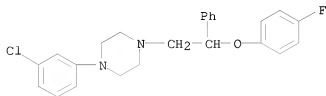
RN 158545-85-8 CAPLUS

CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-
 (CA INDEX NAME)



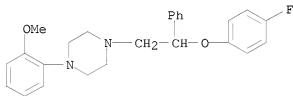
RN 691872-56-7 CAPLUS

CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]- (CA INDEX NAME)



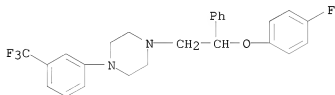
RN 691872-58-9 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



RN 691872-60-3 CAPLUS

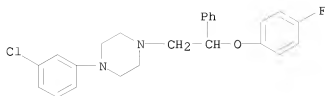
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 691872-62-5 CAPLUS

CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-, hydrochloride (1:1) (CA INDEX NAME)

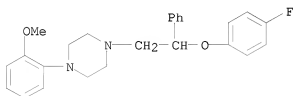
10/513699



● HCl

RN 691872-64-7 CAPLUS

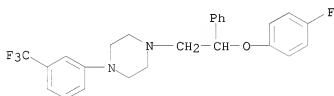
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 691872-66-9 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

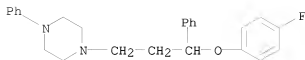


● HCl

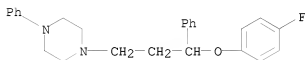
RN 866548-21-2 CAPLUS

CN Piperazine, 1-[3-(4-fluorophenoxy)-3-phenylpropyl]-4-phenyl- (CA INDEX NAME)

10/513699

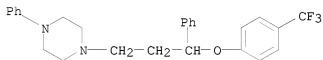


RN 866548-22-3 CAPLUS
CN Piperazine, 1-[3-(4-fluorophenoxy)-3-phenylpropyl]-4-phenyl-,
hydrochloride (1:1) (CA INDEX NAME)



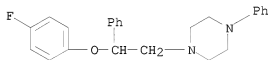
● HCl

RN 866548-23-4 CAPLUS
CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-,
hydrochloride (1:1) (CA INDEX NAME)



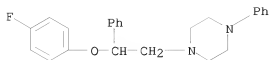
● HCl

RN 866548-24-5 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-phenyl- (CA INDEX
NAME)



RN 866548-25-6 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-phenyl-, hydrochloride
(1:1) (CA INDEX NAME)

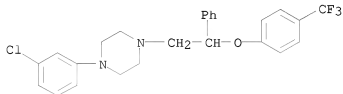
10/513699



● HCl

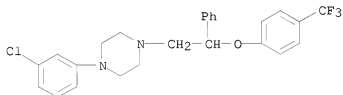
RN 866548-26-7 CAPLUS

CN Piperazine, 1-(3-chlorophenyl)-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]- (CA INDEX NAME)



RN 866548-27-8 CAPLUS

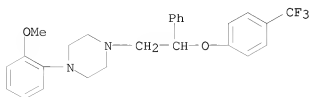
CN Piperazine, 1-(3-chlorophenyl)-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 866548-28-9 CAPLUS

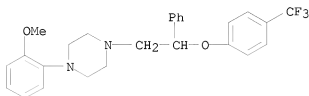
CN Piperazine, 1-(2-methoxyphenyl)-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]- (CA INDEX NAME)



10/513699

RN 866548-29-0 CAPLUS

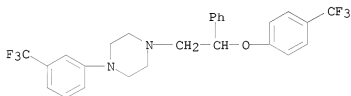
CN Piperazine, 1-(2-methoxyphenyl)-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

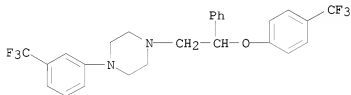
RN 866548-30-3 CAPLUS

CN Piperazine, 1-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 866548-31-4 CAPLUS

CN Piperazine, 1-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

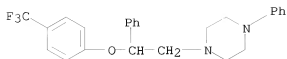


● HCl

RN 866548-36-9 CAPLUS

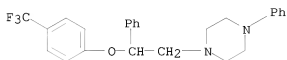
CN Piperazine, 1-phenyl-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]- (CA INDEX NAME)

10/513699



RN 866548-37-0 CAPLUS

CN Piperazine, 1-phenyl-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-,
hydrochloride (1:1) (CA INDEX NAME)



● HCl

L3 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2004:344622 CAPLUS
 DOCUMENT NUMBER: 140:357212
 TITLE: Preparation of substituted anilinic piperidines as MCH selective antagonists
 INVENTOR(S): Marzabadi, Mohammad R.; Wetzel, John; Deleon, John E.; Jiang, Yu; Chen, Chien-An; Lu, Kai
 PATENT ASSIGNEE(S): Synaptic Pharmaceutical Corporation, USA
 SOURCE: U.S., 394 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 6727264 | B1 | 20040427 | US 2002-188434 | 20020703 |
| US 20040073036 | A1 | 20040415 | US 2003-345063 | 20030114 |
| US 20060041139 | A9 | 20060223 | | |
| US 7105544 | B2 | 20060912 | | |
| US 7067534 | B1 | 20060627 | US 2003-719358 | 20031121 |
| US 20040186103 | A1 | 20040923 | US 2004-753057 | 20040106 |
| US 20060084649 | A9 | 20060420 | | |
| US 7199135 | B2 | 20070403 | | |
| US 20060217418 | A1 | 20060928 | US 2005-541991 | 20050705 |
| US 20070043080 | A1 | 20070222 | US 2005-214968 | 20050830 |
| PRIORITY APPLN. INFO.: | | | | |
| | | | US 2001-303091P | P 20010705 |
| | | | US 2002-346997P | P 20020109 |
| | | | US 2002-188434 | A2 20020703 |
| | | | WO 2002-US21063 | A2 20020703 |
| | | | US 2003-345063 | A2 20030114 |
| | | | US 2003-719358 | A1 20031121 |
| | | | WO 2004-US175 | W 20040106 |
| OTHER SOURCE(S): | | | | |
| MARPAT 140:357212 | | | | |
| GI | | | | |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I (R1 = H, alkyl, aryl, etc.; R2 = alkyl, cyclopropyl; R3 = (un)substituted (hetero)aryl; A = H, F, Cl, Br, CN, etc.; X = O, NH; n = 0-5), II (W = III, IV (wherein R1 = H, Me, Et; X = O, NR3, CO, a bond; Y = H, (hetero)aryl; R3 = H, (hetero)aryl); R2 and A as above)] which are selective antagonists for melanin concentrating hormone-1 (MCH1) receptors, were prepared. Thus, reacting 2-methyl-N-[3-(4-piperidinyl)phenyl]propanamide (preparation given) with 4-chloro-3',4'-dimethylbutyrophenone in the presence of K2CO3 and NaI in DMF afforded 80% V which showed Ki of 3.9 nM in cloned rat MCH1 binding assay.

IT 387826-65-5P 387826-66-6P 387826-67-7P
 387826-68-8P 387826-69-9P 387826-73-5P
 387826-74-6P 387826-79-1P 387826-80-4P
 387826-81-5P 387826-82-6P 387826-85-9P
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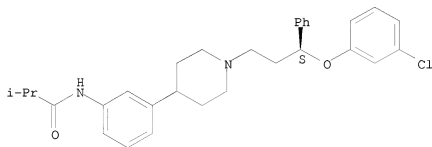
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted anilinic piperidines as MCH selective antagonists)

RN 387826-65-5 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(3-chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

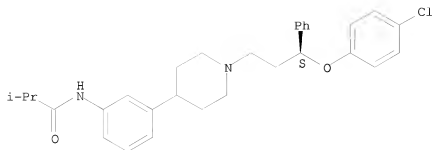
Absolute stereochemistry.



RN 387826-66-6 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(4-chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

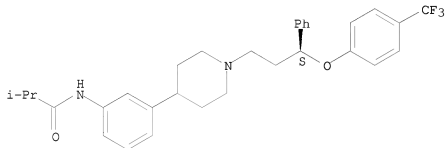
Absolute stereochemistry.



RN 387826-67-7 CAPLUS

CN Propanamide, 2-methyl-N-[3-[1-[(3S)-3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-piperidinyl]phenyl]- (CA INDEX NAME)

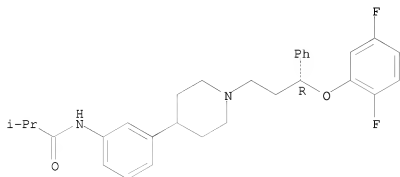
Absolute stereochemistry.



RN 387826-68-8 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-(2,5-difluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

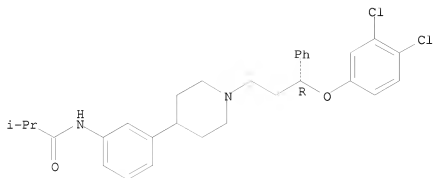


RN 387826-69-9 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-(3,4-dichlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

10/513699

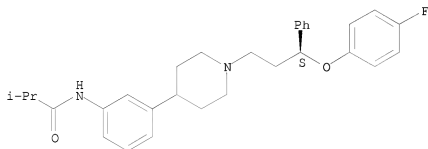
Absolute stereochemistry.



RN 387826-73-5 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(4-fluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

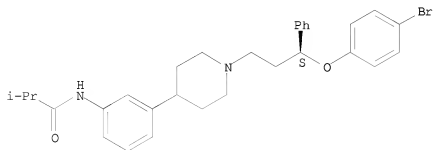
Absolute stereochemistry.



RN 387826-74-6 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(4-bromophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 387826-79-1 CAPLUS

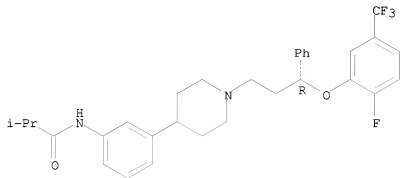
<12/04/2007>

Erich Leese

10/513699

CN Propanamide, N-[3-[1-[(3R)-3-[2-fluoro-5-(trifluoromethyl)phenoxy]-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

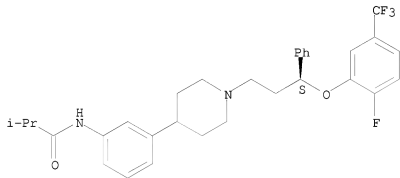
Absolute stereochemistry.



RN 387826-80-4 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-[2-fluoro-5-(trifluoromethyl)phenoxy]-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

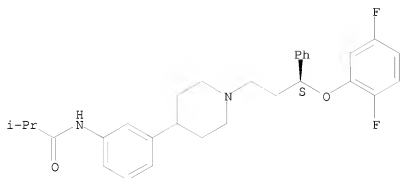
Absolute stereochemistry.



RN 387826-81-5 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(2,5-difluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

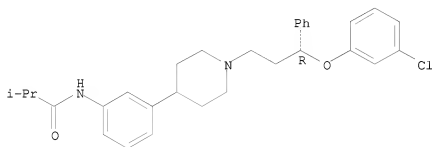
Absolute stereochemistry.



RN 387826-82-6 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-(3-chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

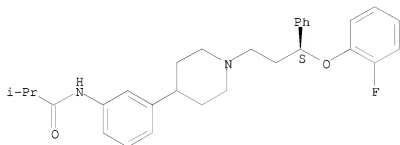
Absolute stereochemistry.



RN 387826-85-9 CAPLUS

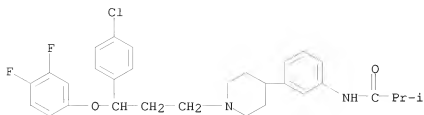
CN Propanamide, N-[3-[1-[(3S)-3-(2-fluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.



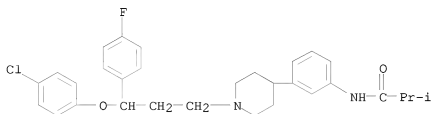
RN 487049-74-1 CAPLUS

CN Propanamide, N-[3-[1-[3-(4-chlorophenyl)-3-(3,4-difluorophenoxy)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



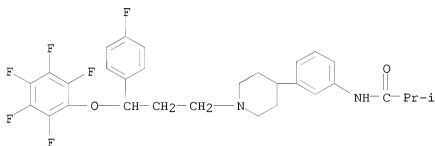
RN 487049-80-9 CAPLUS

CN Propanamide, N-[3-[1-[3-(4-chlorophenoxy)-3-(4-fluorophenyl)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



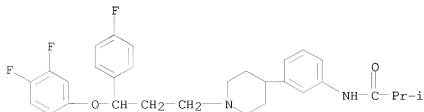
RN 487049-81-0 CAPLUS

CN Propanamide, N-[3-[1-[3-(4-fluorophenyl)-3-(2,3,4,5,6-pentafluorophenoxy)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



RN 487049-83-2 CAPLUS

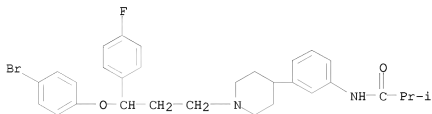
CN Propanamide, N-[3-[1-[3-(3,4-difluorophenoxy)-3-(4-fluorophenyl)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



10/513699

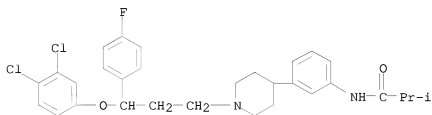
RN 487049-84-3 CAPLUS

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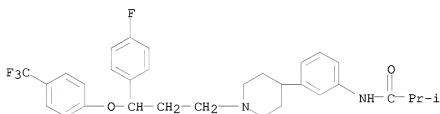
RN 487049-85-4 CAPLUS

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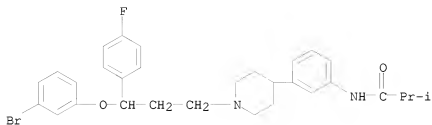
RN 487049-86-5 CAPLUS

CN Propanamide, N-[3-[1-[3-(4-fluorophenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



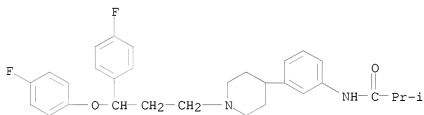
RN 487049-87-6 CAPLUS

CN Propanamide, N-[3-[1-[3-(3-bromophenoxy)-3-(4-fluorophenyl)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



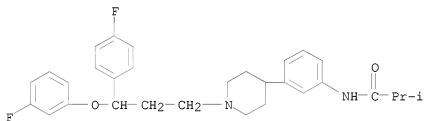
RN 487049-88-7 CAPLUS

CN Propanamide, N-[3-[1-[3-(4-fluorophenoxy)-3-(4-fluorophenyl)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



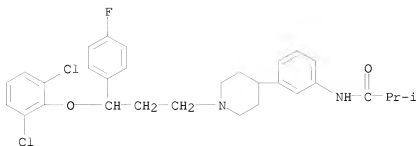
RN 487049-89-8 CAPLUS

CN Propanamide, N-[3-[1-[3-(3-fluorophenoxy)-3-(4-fluorophenyl)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



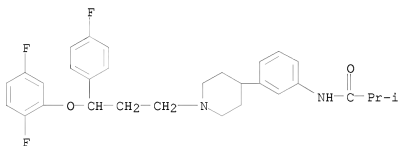
RN 487049-90-1 CAPLUS

CN Propanamide, N-[3-[1-[3-(2,6-dichlorophenoxy)-3-(4-fluorophenyl)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



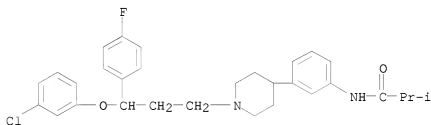
RN 487049-91-2 CAPLUS

CN Propanamide, N-[3-[1-[3-(2,5-difluorophenoxy)-3-(4-fluorophenyl)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



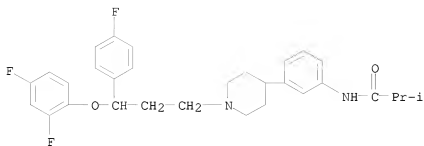
RN 487049-92-3 CAPLUS

CN Propanamide, N-[3-[1-[3-(3-chlorophenoxy)-3-(4-fluorophenyl)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



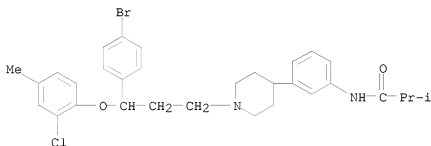
RN 487049-95-6 CAPLUS

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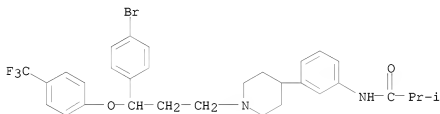
RN 487049-99-0 CAPLUS

CN Propanamide, N-[3-[1-[3-(4-bromophenyl)-3-(2-chloro-4-methylphenoxy)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



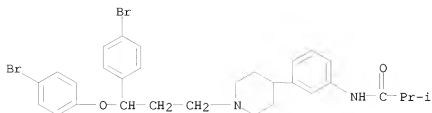
RN 487050-01-1 CAPLUS

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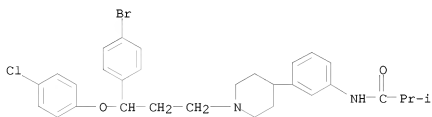
RN 487050-07-7 CAPLUS

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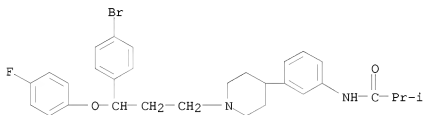
RN 487050-08-8 CAPLUS

CN Propanamide, N-[3-[1-[3-(4-bromophenyl)-3-(4-chlorophenoxy)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



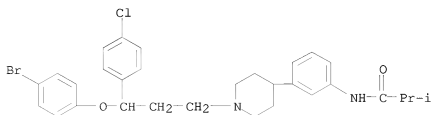
RN 487050-09-9 CAPLUS

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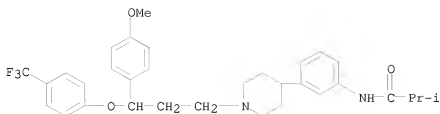


RN 487050-20-4 CAPLUS

CN Propanamide, N-[3-[1-[3-(4-bromophenoxy)-3-(4-chlorophenyl)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

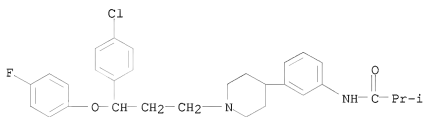


RN 487050-22-6 CAPLUS



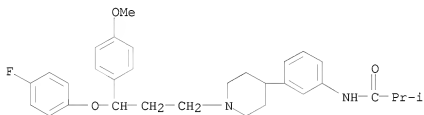
RN 487050-35-1 CAPLUS

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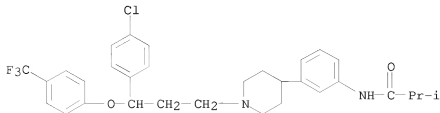
RN 487050-36-2 CAPLUS

CN Propanamide, N-[3-[1-[3-(4-fluorophenoxy)-3-(4-methoxyphenyl)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



RN 487050-39-5 CAPLUS

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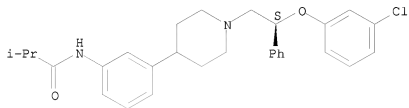


10/513699

RN 487051-81-0 CAPLUS

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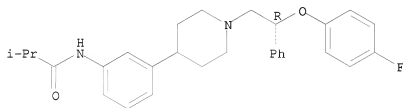
Absolute stereochemistry.



RN 487051-83-2 CAPLUS

CN Propanamide, N-[3-[1-[(2R)-2-(4-fluorophenoxy)-2-phenylethyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

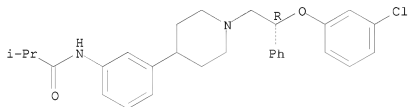
Absolute stereochemistry.



RN 487051-85-4 CAPLUS

CN Propanamide, N-[3-[1-[(2R)-2-(3-chlorophenoxy)-2-phenylethyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

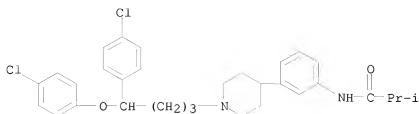
Absolute stereochemistry.



RN 487052-31-3 CAPLUS

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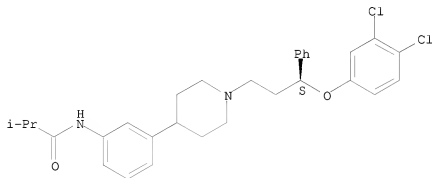
10/513699



RN 487056-49-5 CAPLUS

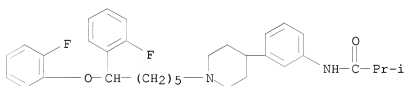
CN Propanamide, N-[3-[1-[(3S)-3-(3,4-dichlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.



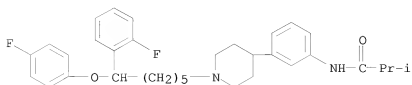
RN 487057-25-0 CAPLUS

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RN 487057-26-1 CAPLUS

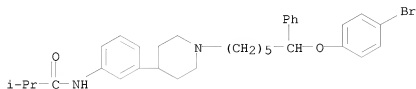
CN Propanamide, N-[3-[1-[6-(4-fluorophenoxy)-6-(2-fluorophenyl)hexyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



10/513699

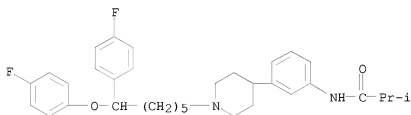
RN 487057-32-9 CAPLUS

CN Propanamide, N-[3-[1-[6-(4-bromophenoxy)-6-phenylhexyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



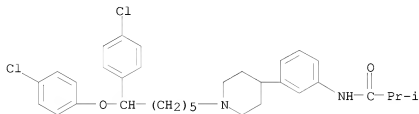
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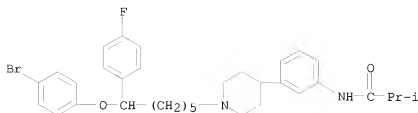
RN 487057-35-2 CAPLUS

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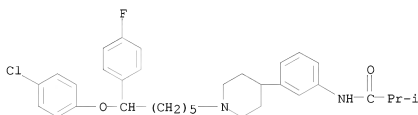
RN 487057-36-3 CAPLUS

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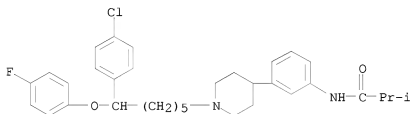
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CN Propanamide, N-[3-[1-[6-(4-chlorophenoxy)-6-(4-fluorophenyl)hexyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



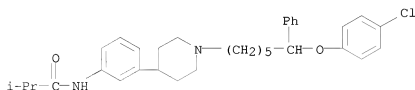
RN 487057-38-5 CAPLUS

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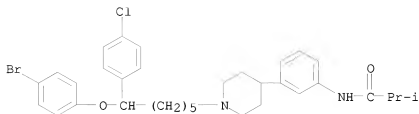
RN 487057-40-9 CAPLUS

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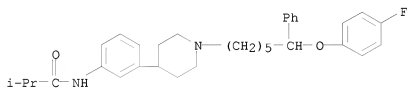
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CN Propanamide, N-[3-[1-[6-(4-bromophenoxy)-6-(4-chlorophenyl)hexyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



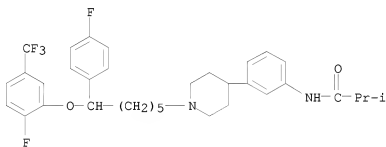
RN 487057-45-4 CAPLUS

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RN 487057-47-6 CAPLUS

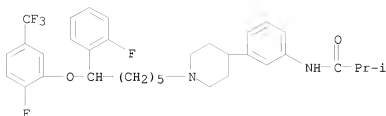
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RN 487057-49-8 CAPLUS

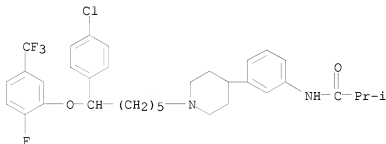
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10/513699



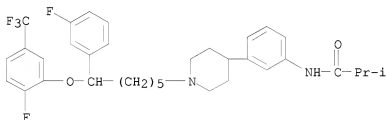
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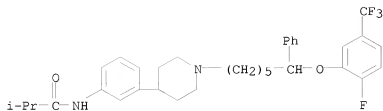
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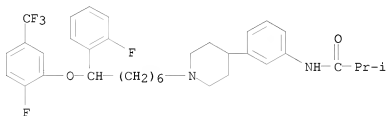
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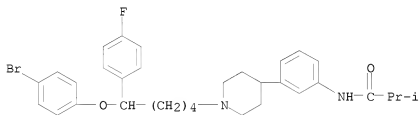
RN 487057-53-4 CAPLUS

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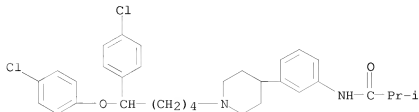
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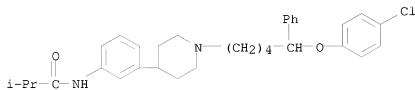
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10/513699

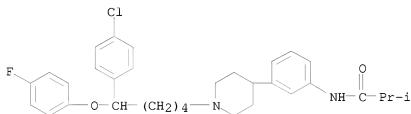
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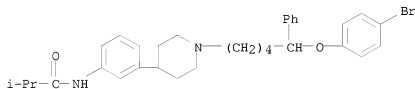
RN 487057-59-0 CAPLUS

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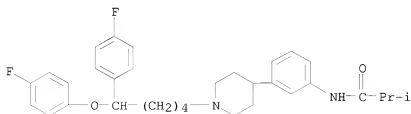
RN 487057-60-3 CAPLUS

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RN 487057-62-5 CAPLUS

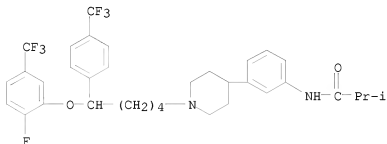
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RN 487057-65-8 CAPLUS

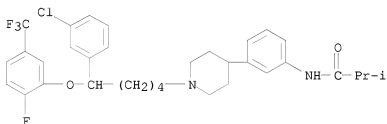
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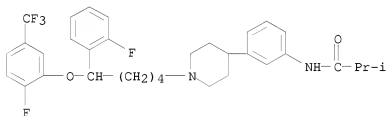
RN 487057-66-9 CAPLUS

CN Propanamide, N-[3-[1-[5-(3-chlorophenyl)-5-[2-fluoro-5-(trifluoromethyl)phenoxy]pentyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



RN 487057-67-0 CAPLUS

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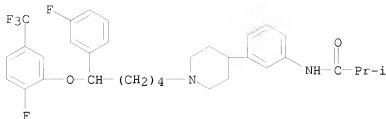


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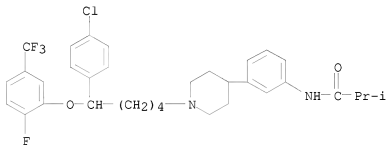
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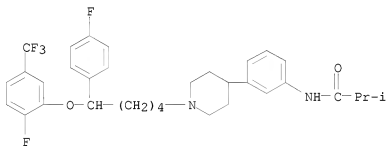
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RN 487057-70-5 CAPLUS
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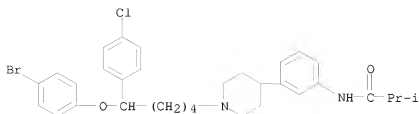


RN 487057-71-6 CAPLUS
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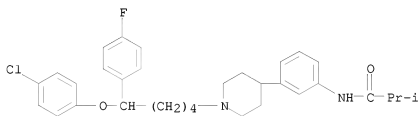
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10/513699



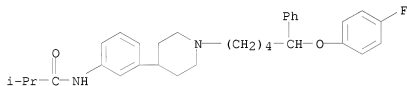
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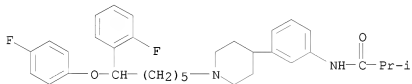
RN 487057-76-1 CAPLUS

CN Propanamide, N-[3-[1-[5-(4-fluorophenoxy)-5-phenylpentyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



RN 488098-61-9 CAPLUS

CN Propanamide, N-[3-[1-[6-(4-fluorophenoxy)-6-(2-fluorophenyl)hexyl]-4-piperidinyl]phenyl]-2-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

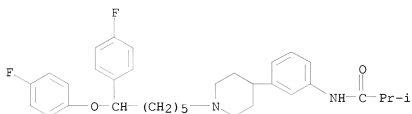
RN 488098-62-0 CAPLUS

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Erich Leese

10/513699

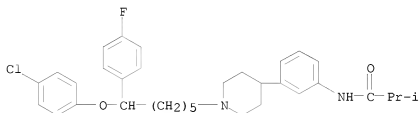
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● HCl

RN 488098-63-1 CAPLUS

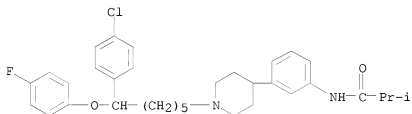
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● HCl

RN 488098-64-2 CAPLUS

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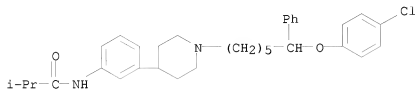


● HCl

RN 488098-65-3 CAPLUS

10/513699

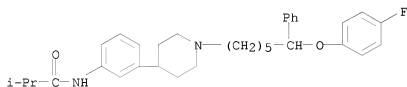
CN Propanamide, N-[3-[1-[6-(4-chlorophenoxy)-6-phenylhexyl]-4-piperidinyl]phenyl]-2-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 488098-67-5 CAPLUS

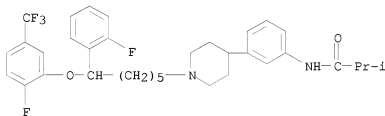
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● HCl

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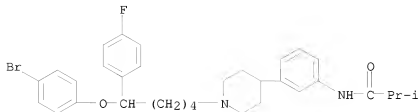
CN Propanamide, N-[3-[1-[6-(2-fluorophenyl)-6-[2-fluoro-5-(trifluoromethyl)phenoxy]hexyl]-4-piperidinyl]phenyl]-2-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 488098-70-0 CAPLUS

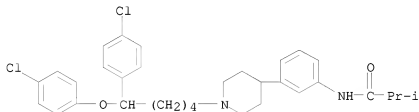
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● HCl

RN 488098-71-1 CAPLUS

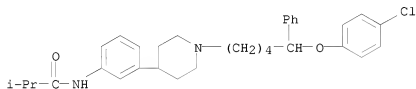
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● HCl

RN 488098-72-2 CAPLUS

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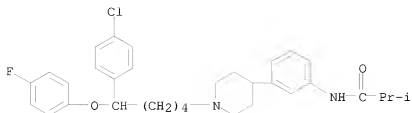


● HCl

RN 488098-73-3 CAPLUS

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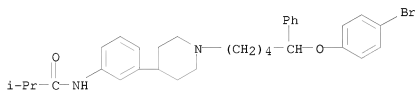
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● HCl

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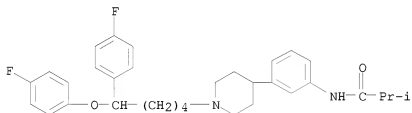
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● HCl

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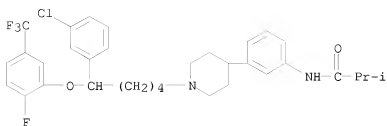


● HCl

RN 488098-77-7 CAPLUS

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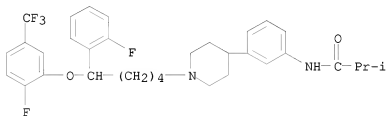
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● HCl

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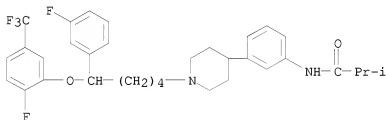
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● HCl

RN 488098-79-9 CAPLUS

CN Propanamide, N-[3-[1-[5-(3-fluorophenyl)-5-[2-fluoro-5-(trifluoromethyl)phenoxy]pentyl]-4-piperidinyl]phenyl]-2-methyl-, hydrochloride (1:1) (CA INDEX NAME)

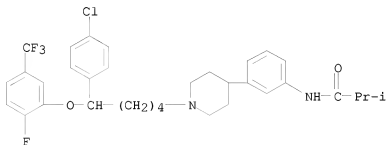


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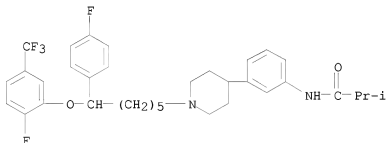
CN Propanamide, N-[3-[1-[5-(4-chlorophenyl)-5-[2-fluoro-5-(trifluoromethyl)phenoxy]pentyl]-4-piperidinyl]phenyl]-2-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 488098-82-4 CAPLUS

CN Propanamide, N-[3-[1-[6-(4-fluorophenyl)-6-[2-fluoro-5-(trifluoromethyl)phenoxy]hexyl]-4-piperidinyl]phenyl]-2-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

REFERENCE COUNT:

25

THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:170822 CAPLUS

DOCUMENT NUMBER: 140:417233

TITLE: Synthesis and biological evaluation of 2-(4-fluorophenoxy)-2-phenyl-ethyl piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile
 AUTHOR(S): Dorsey, James M.; Miranda, Maria G.; Cozzi, Nicholas V.; Pinney, Kevin G.

CORPORATE SOURCE: Department of Chemistry and Biochemistry and The Center for Drug Discovery, Baylor University, Waco, TX, 76798-7348, USA

SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(6), 1483-1491

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:417233

AB Three new 2-(4-fluorophenoxy)-2-phenyl-Et piperazines, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-piperazine, and 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(3-trifluoromethylphenyl)-piperazine, modeled after the potent antidepressant fluoxetine and coupled with several functionalized piperazines, have been prepared by chemical synthesis as selective serotonin reuptake inhibitors (SSRIs) with a potentially improved adverse reaction profile. Typical SSRIs, although very effective in the treatment of depression, still face the troublesome side effect of sexual dysfunction. A number of pharmacol. agents-notably, drugs in the piperazine class-have been used to reverse SSRI-induced sexual dysfunction, and evidence for developing an improved SSRI by coupling a fluoxetine congener with the pharmacophore of a reversal agent holds promise. Preliminary data indicates that the hydrochloride (HCl) salts of piperazines exhibit single-site binding at the site of the serotonin reuptake transporter (SERT). However, each of the three compds. are much less potent than typical SSRIs, showing micromolar (μM) affinity for the SERT with IC_{50} values of 1.45 μM , 3.27 μM , and 9.56 μM , resp. Further biol. evaluation of piperazine compds. is needed before definitive conclusions can be made with regard to each compound's potential for use as an SSRI-type candidate which is devoid of sexual side effects. Nevertheless, the initial findings are quite encouraging, thus lending credence to the idea of hybridizing an SSRI congener with that of the pharmacophore of an agent known to reverse or treat SSRI-induced sexual dysfunction.

IT 691872-62-5P 691872-64-7P 691872-66-9P

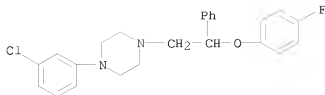
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis and structure-activity relationship of 2-(4-fluorophenoxy)-2-Ph-Et piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile)

RN 691872-62-5 CAPLUS

CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-, hydrochloride (1:1) (CA INDEX NAME)

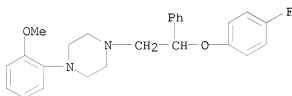
10/513699



● HCl

RN 691872-64-7 CAPLUS

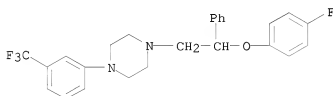
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 691872-66-9 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

IT 691872-56-7P 691872-58-9P 691872-60-3P

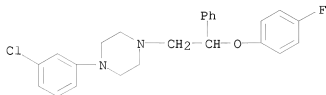
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and structure-activity relationship of 2-(4-fluorophenoxy)-2-Ph-Et piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile)

RN 691872-56-7 CAPLUS

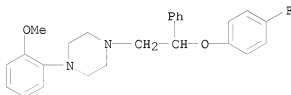
10/513699

CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]- (CA INDEX NAME)



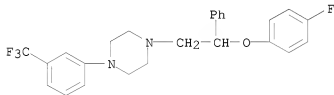
RN 691872-58-9 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



RN 691872-60-3 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



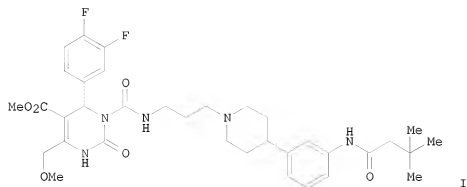
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:162444 CAPLUS
 DOCUMENT NUMBER: 140:212060
 TITLE: DNA encoding a human melanin concentrating hormone receptor (MCH1) and uses thereof and preparation of 4-phenylpiperidine derivatives as human MCH1 receptor antagonists
 INVENTOR(S): Salon, John A.; Laz, Thomas M.; Nagorny, Raisa; Wilson, Amy E.; Craig, Douglas A.
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 180 pp., Cont.-in-part of U.S. Ser. No. 899,732.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|-----------------|-------------|
| US 20040038855 | A1 | 20040226 | US 2003-341751 | 20030114 |
| WO 2000039279 | A2 | 20000706 | WO 1999-US31169 | 19991230 |
| WO 2000039279 | A3 | 20001102 | | |
| W: | AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW | | | |
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| US 20030082623 | A1 | 20030501 | US 2001-899732 | 20010705 |
| WO 2004064774 | A2 | 20040805 | WO 2004-US724 | 20040114 |
| WO 2004064774 | A3 | 20061005 | | |
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| PRIORITY APPLN. INFO.: | | | WO 1999-US31169 | A2 19991230 |
| | | | US 2000-610635 | B2 20000705 |
| | | | US 2001-899732 | A2 20010705 |
| | | | US 1998-224426 | A2 19981231 |
| | | | US 2003-341751 | A 20030114 |

GI



AB This invention provides an isolated nucleic acid encoding a human MCH1 receptor, a purified human MCH1 receptor, vectors comprising isolated nucleic acid encoding a human MCH1 receptor, cells comprising such vectors, antibodies directed to a human MCH1 receptor, nucleic acid probes useful for detecting nucleic acid encoding human MCH1 receptors, antisense oligonucleotides complementary to unique sequences of nucleic acid encoding human MCH1 receptors, transgenic, nonhuman animals which express DNA encoding a normal or mutant human MCH1 receptor, methods of isolating a human MCH1 receptor, methods of treating an abnormality that is linked to the activity of a human MCH1 receptor, as well as methods of determining binding of compds. to mammalian MCH1 receptors. This invention further provides a method of treating a subject suffering from urinary incontinence which comprises administering to the subject an amount of an MCH1 antagonist effective to treat the subject's urinary incontinence or overactive bladder. Various 4-phenylpiperidine derivs., e.g (I), were synthesized and tested as human MCH1 receptor antagonists.

IT 387826-65-5P, N-[3-[1-[(3S)-3-(3-Chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methylpropanamide 387826-66-6P, N-[3-[1-[(3S)-3-(4-Chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methylpropanamide 387826-67-7P, 2-Methyl-N-[3-[1-[(3S)-3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-piperidinyl]phenyl]propanamide 387826-68-8P, N-[3-[1-[(3R)-3-(2,5-Difluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methylpropanamide 387826-69-9P, N-[3-[1-[(3R)-3-(3,4-Dichlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methylpropanamide 387826-73-5P, N-[3-[1-[(3S)-3-(4-Fluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methylpropanamide 387826-74-6P, N-[3-[1-[(3S)-3-(4-Bromophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methylpropanamide 387826-79-1P, N-[3-[1-[(3R)-3-[2-Fluoro-5-(trifluoromethyl)phenoxy]-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methylpropanamide 387826-80-4P, N-[3-[1-[(3S)-3-[2-Fluoro-5-(trifluoromethyl)phenoxy]-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methylpropanamide 387826-81-5P, N-[3-[1-[(3S)-3-(2,5-Difluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methylpropanamide 387826-82-6P, N-[3-[1-[(3R)-3-(3-Chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methylpropanamide 387826-85-9P, N-[3-[1-[(3S)-3-(2-Fluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methylpropanamide

10/513699

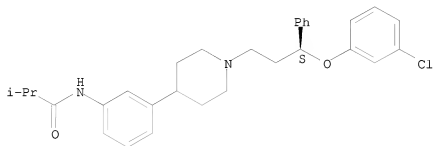
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(DNA encoding human melanin concentrating hormone receptor (MCH1) and uses thereof and preparation of phenylpiperidine derivs. as human MCH1 antagonists)

RN 387826-65-5 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(3-chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

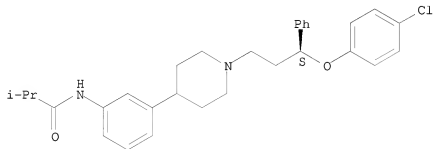
Absolute stereochemistry.



RN 387826-66-6 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(4-chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

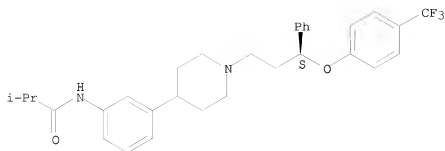
Absolute stereochemistry.



RN 387826-67-7 CAPLUS

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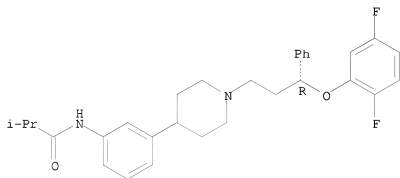
Absolute stereochemistry.



RN 387826-68-8 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-(2,5-difluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

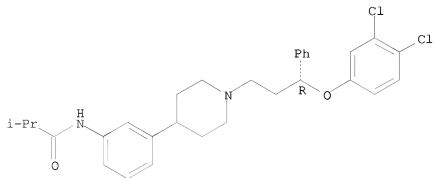
Absolute stereochemistry.



RN 387826-69-9 CAPLUS

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Absolute stereochemistry.

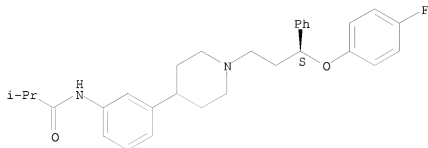


RN 387826-73-5 CAPLUS

10/513699

CN Propanamide, N-[3-[1-[(3S)-3-(4-fluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

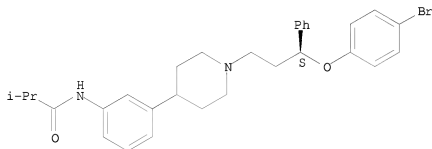
Absolute stereochemistry.



RN 387826-74-6 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(4-bromophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

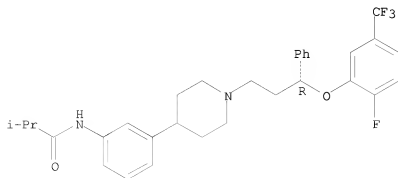
Absolute stereochemistry.



RN 387826-79-1 CAPLUS

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Absolute stereochemistry.

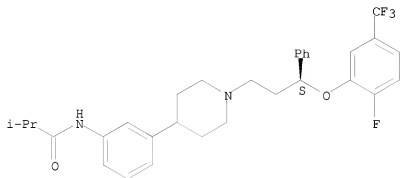


10/513699

RN 387826-80-4 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-[2-fluoro-5-(trifluoromethyl)phenoxy]-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

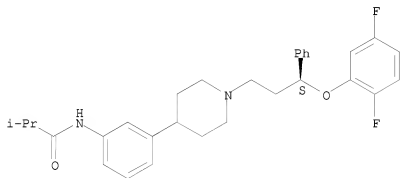
Absolute stereochemistry.



RN 387826-81-5 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(2,5-difluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

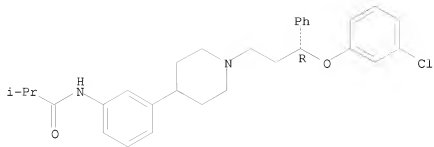


RN 387826-82-6 CAPLUS

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Absolute stereochemistry.

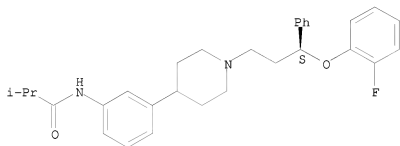
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RN 387826-85-9 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(2-fluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:334519 CAPLUS

DOCUMENT NUMBER: 138:298124

TITLE: Human melanin concentrating hormone receptor MCH1, its DNA, its synthetic ligands and diagnostic and therapeutic uses thereof

INVENTOR(S): Borowsky, Beth; Blackburn, Thomas P.; Ogozalek, Kristine

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 193 pp., Cont.-in-part of U.S. Ser. No. 610,635.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|--|--------------|-----------------|-------------|
| US 20030082623 | A1 | 20030501 | US 2001-899732 | 20010705 |
| US 6221613 | B1 | 20010424 | US 1998-224426 | 19981231 |
| WO 2000039279 | A2 | 20000706 | WO 1999-US31169 | 19991230 |
| WO 2000039279 | A3 | 20001102 | | |
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| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 20030077701 | A1 | 20030424 | US 2001-29314 | 20011220 |
| US 20040038855 | A1 | 20040226 | US 2003-341751 | 20030114 |
| PRIORITY APPLN. INFO.: | | | | |
| | | | US 1998-224426 | A2 19981231 |
| | | | WO 1999-US31169 | A2 19991230 |
| | | | US 2000-610635 | A2 20000705 |
| | | | US 2001-899732 | A1 20010705 |
| AB | This invention provides an isolated nucleic acid encoding a human MCH1 receptor, a purified human MCH1 receptor, vectors comprising isolated nucleic acid encoding a human MCH1 receptor, cells comprising such vectors, antibodies directed to a human MCH1 receptor, nucleic acid probes useful for detecting nucleic acid encoding human MCH1 receptors, antisense oligonucleotides complementary to unique sequences of nucleic acid encoding human MCH1 receptors, transgenic, nonhuman animals which express DNA encoding a normal or mutant human MCH1 receptor, methods of isolating a human MCH1 receptor, methods of treating an abnormality that is linked to the activity of a human MCH1 receptor, as well as methods of determining binding of compds. to mammalian MCH1 receptors. This invention provides a method of modifying the feeding behavior of a subject which comprises administering to the subject an amount of an MCH1 antagonist effective to decrease the body mass of the subject and/or decrease the consumption of food by the subject. This invention further provides a method of treating a subject suffering from depression and/or anxiety which comprises administering to the subject an amount of an MCH1 antagonist effective to treat the subject's depression and/or anxiety. | | | |
| IT | 387826-65-5P | 387826-66-6P | 387826-67-7P | |
| | 387826-68-8P | 387826-69-9P | 387826-73-5P | |

10/513699

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387826-81-5P 387826-82-6P 387826-85-9P

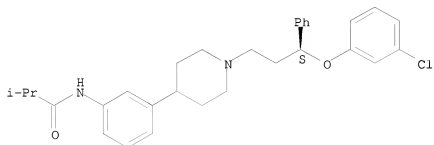
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(human melanin concentrating hormone receptor MCH1, its DNA, its synthetic ligands and diagnostic and therapeutic uses thereof)

RN 387826-65-5 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(3-chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

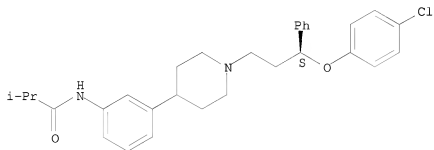
Absolute stereochemistry.



RN 387826-66-6 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(4-chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

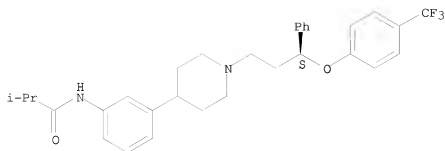
Absolute stereochemistry.



RN 387826-67-7 CAPLUS

CN Propanamide, 2-methyl-N-[3-[1-[(3S)-3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-piperidinyl]phenyl]- (CA INDEX NAME)

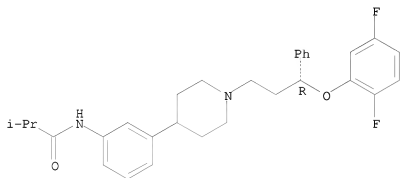
Absolute stereochemistry.



RN 387826-68-8 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-(2,5-difluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

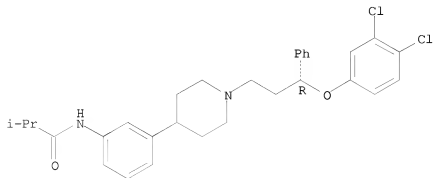
Absolute stereochemistry.



RN 387826-69-9 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-(3,4-dichlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

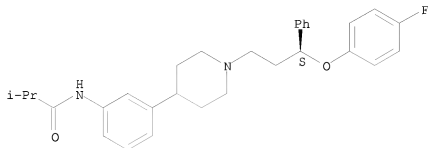


RN 387826-73-5 CAPLUS

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CN Propanamide, N-[3-[1-[(3S)-3-(4-fluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

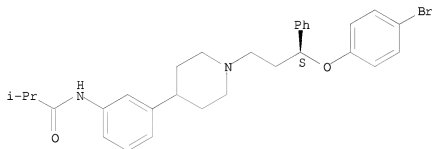
Absolute stereochemistry.



RN 387826-74-6 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(4-bromophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

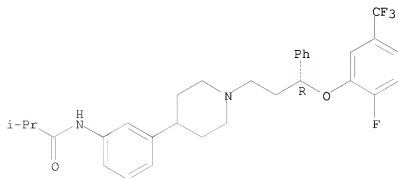
Absolute stereochemistry.



RN 387826-79-1 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-[2-fluoro-5-(trifluoromethyl)phenoxy]-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

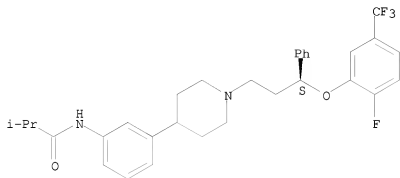


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RN 387826-80-4 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-[2-fluoro-5-(trifluoromethyl)phenoxy]-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

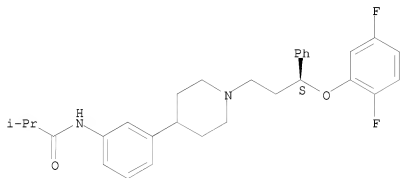
Absolute stereochemistry.



RN 387826-81-5 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(2,5-difluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

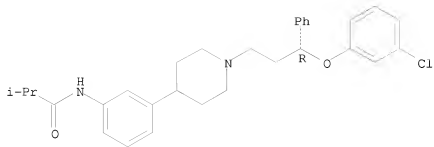


RN 387826-82-6 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-(3-chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

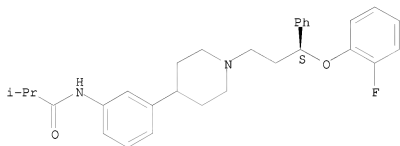
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RN 387826-85-9 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(2-fluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

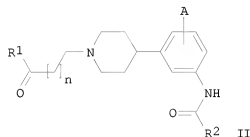
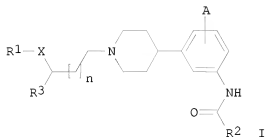


L3 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2003:42108 CAPLUS
 DOCUMENT NUMBER: 138:106601
 TITLE: Preparation of substituted anilinic piperidines as MCH selective antagonists
 INVENTOR(S): Marzabadi, Mohammad R.; Wetzel, John; Deleon, John E.; Jiang, Yu
 PATENT ASSIGNEE(S): Synaptic Pharmaceutical Corporation, USA
 SOURCE: PCT Int. Appl., 7/1 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|-------------|
| WO 2003004027 | A1 | 20030116 | WO 2002-US21063 | 20020703 |
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| AU 2002316531 | A1 | 20030121 | AU 2002-316531 | 20020703 |
| AU 2002316531 | B2 | 20070913 | | |
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| BR 2002010869 | A | 20040629 | BR 2002-10869 | 20020703 |
| JP 2004536104 | T | 20041202 | JP 2003-510038 | 20020703 |
| HU 2004001880 | A2 | 20050128 | HU 2004-1880 | 20020703 |
| ZA 2003009860 | A | 20050311 | ZA 2003-9860 | 20020703 |
| CN 1671386 | A | 20050921 | CN 2002-817212 | 20020703 |
| NZ 530221 | A | 20060331 | NZ 2002-530221 | 20020703 |
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| US 7105544 | B2 | 20060912 | | |
| MX 2003011886 | A | 20050307 | MX 2003-11886 | 20031218 |
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| US 20040186103 | A1 | 20040923 | US 2004-753057 | 20040106 |
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| US 7199135 | B2 | 20070403 | | |
| IN 2004CN00230 | A | 20051209 | IN 2004-CN230 | 20040205 |
| PRIORITY APPLN. INFO.: | | | US 2001-899794 | A 20010705 |
| | | | US 2002-42582 | A 20020109 |
| | | | US 2001-303091P | P 20010705 |
| | | | US 2002-346997P | P 20020109 |
| | | | US 2002-188434 | A2 20020703 |
| | | | WO 2002-US21063 | W 20020703 |
| | | | US 2003-345063 | A2 20030114 |

OTHER SOURCE(S): MARPAT 138:106601

GI



AB The title compds. [I (R1 = H, alkyl, aryl, etc.; R2 = alkyl, cyclopropyl; R3 = (un)substituted (hetero)aryl; A = H, F, Cl, Br, CN, etc.; X = O, NH; n = 0-5), II (R1 = (un)substituted (hetero)aryl; R2, A, n as above), etc.] which are selective antagonists for melanin concentrating hormone-1 (MCH1)

receptors, were prepared and formulated. Thus, reacting 2-methyl-N-[3-(4-piperidinyl)phenyl]propanamide (preparation given) with 4-chloro-3',4'-dimethylbutyrophenone in the presence of K2CO3 and NaI in DMF afforded 80% II [R1 = R1 = 3,4-Me2C6H3; R2 = iso-Pr; A = H; n = 2] which showed Ki of 3.9 nM in cloned rat MCH1 binding assay.

IT 387826-65-5P 387826-66-6P 387826-67-7P
 387826-68-8P 387826-69-9P 387826-73-5P
 387826-74-6P 387826-79-1P 387826-80-4P
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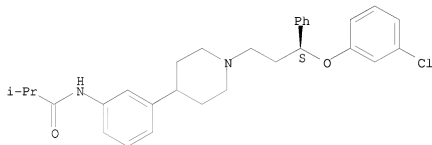
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted anilinic piperidines as MCH selective antagonists)

RN 387826-65-5 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(3-chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

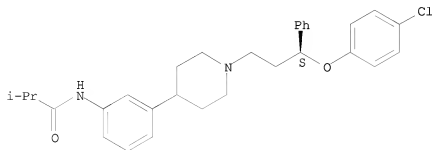
Absolute stereochemistry.



RN 387826-66-6 CAPLUS

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Absolute stereochemistry.

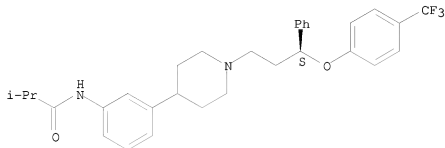


RN 387826-67-7 CAPLUS

10/513699

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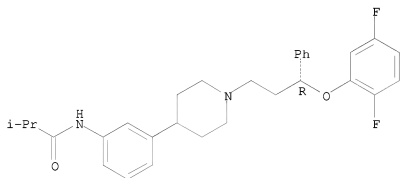
Absolute stereochemistry.



RN 387826-68-8 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-(2,5-difluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

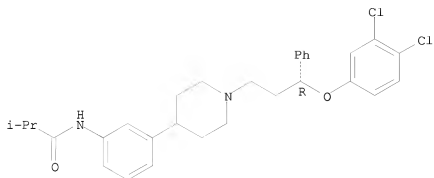
Absolute stereochemistry.



RN 387826-69-9 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-(3,4-dichlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

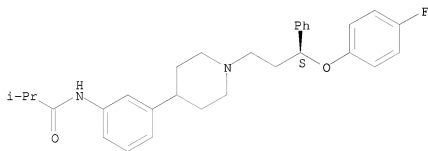
Absolute stereochemistry.



RN 387826-73-5 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(4-fluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

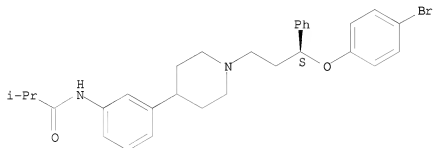
Absolute stereochemistry.



RN 387826-74-6 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(4-bromophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

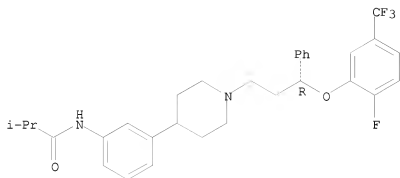


RN 387826-79-1 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-[2-fluoro-5-(trifluoromethyl)phenoxy]-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

10/513699

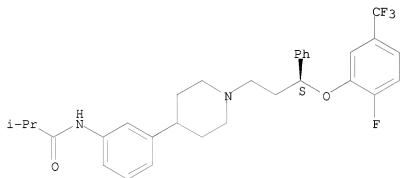
Absolute stereochemistry.



RN 387826-80-4 CAPLUS

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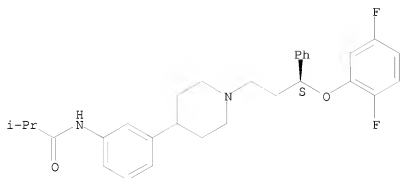
Absolute stereochemistry.



RN 387826-81-5 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(2,5-difluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

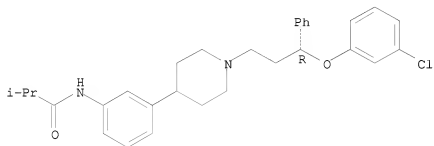
Absolute stereochemistry.



RN 387826-82-6 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-(3-chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

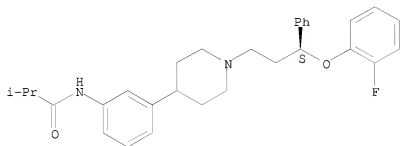
Absolute stereochemistry.



RN 387826-85-9 CAPLUS

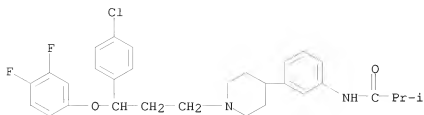
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Absolute stereochemistry.



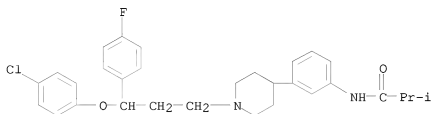
RN 487049-74-1 CAPLUS

CN Propanamide, N-[3-[1-[3-(4-chlorophenyl)-3-(3,4-difluorophenoxy)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



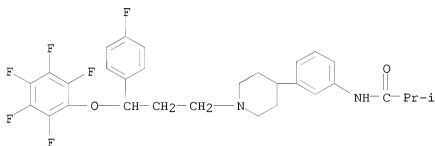
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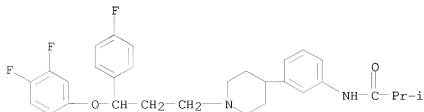
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CN Propanamide, N-[3-[1-[3-(4-fluorophenyl)-3-(2,3,4,5,6-pentafluorophenoxy)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



RN 487049-83-2 CAPLUS

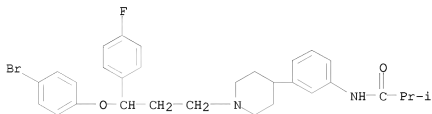
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10/513699

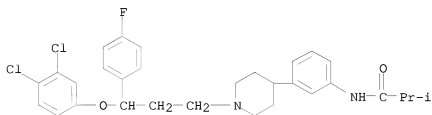
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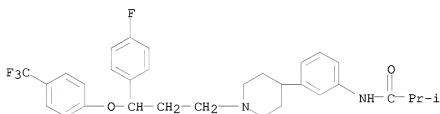
RN 487049-85-4 CAPLUS

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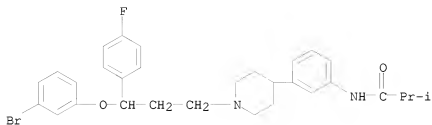
RN 487049-86-5 CAPLUS

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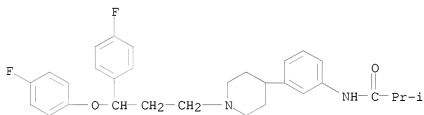
RN 487049-87-6 CAPLUS

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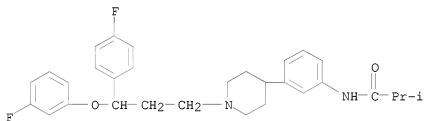
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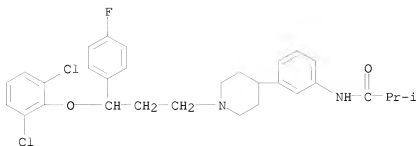
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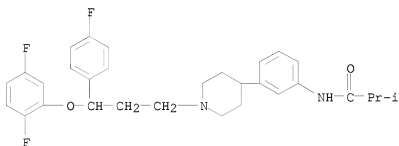
RN 487049-90-1 CAPLUS

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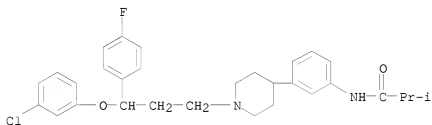
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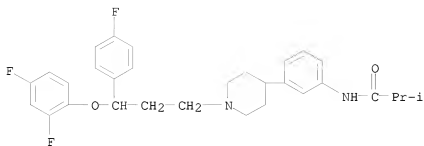
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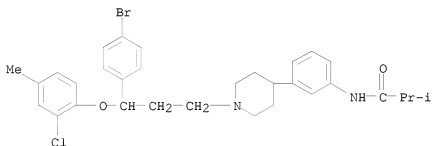
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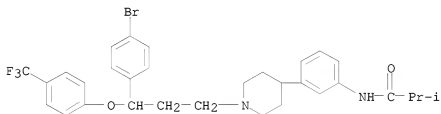
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CN Propanamide, N-[3-[1-[3-(4-bromophenyl)-3-(2-chloro-4-methylphenoxy)propyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



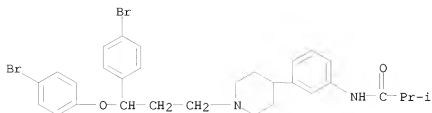
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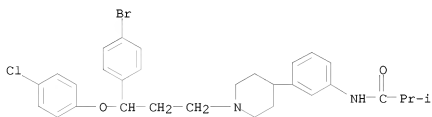
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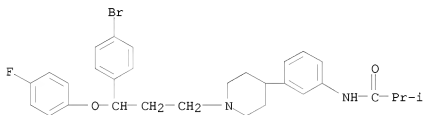
RN 487050-08-8 CAPLUS

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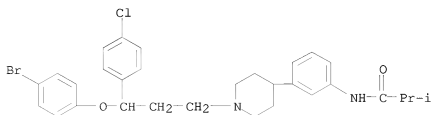
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RN 487050-20-4 CAPLUS

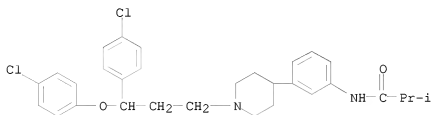
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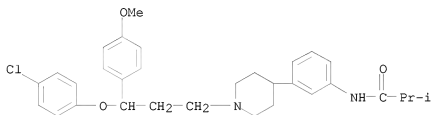
10/513699

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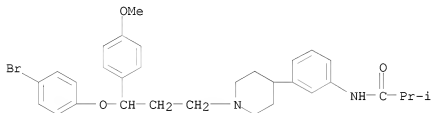
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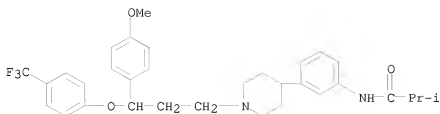
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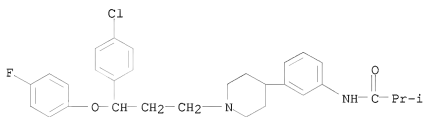
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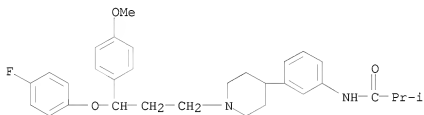
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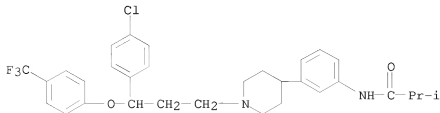
RN 487050-36-2 CAPLUS

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RN 487050-39-5 CAPLUS

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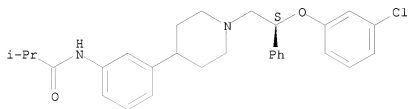


10/513699

RN 487051-81-0 CAPLUS

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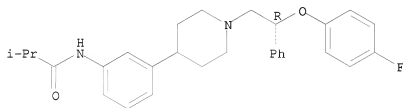
Absolute stereochemistry.



RN 487051-83-2 CAPLUS

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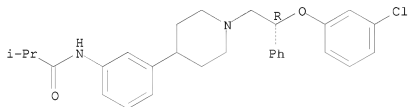
Absolute stereochemistry.



RN 487051-85-4 CAPLUS

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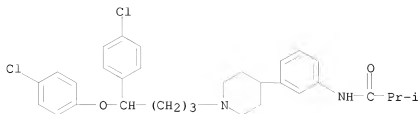
Absolute stereochemistry.



RN 487052-31-3 CAPLUS

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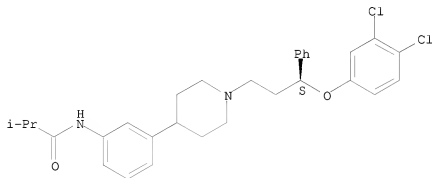
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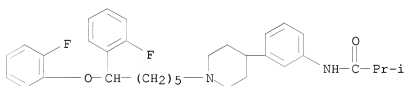
CN Propanamide, N-[3-[1-[(3S)-3-(3,4-dichlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.



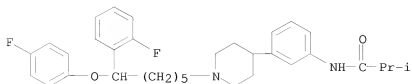
RN 487057-25-0 CAPLUS

CN Propanamide, N-[3-[1-[6-(2-fluorophenoxy)-6-(2-fluorophenyl)hexyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



RN 487057-26-1 CAPLUS

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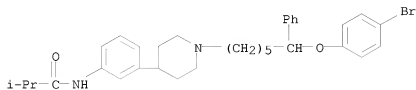
<12/04/2007>

Erich Leese

10/513699

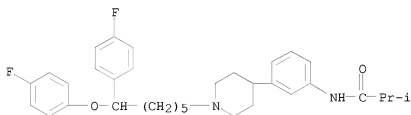
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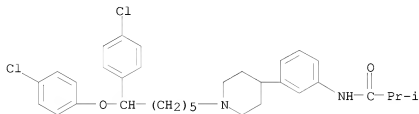
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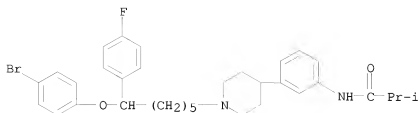
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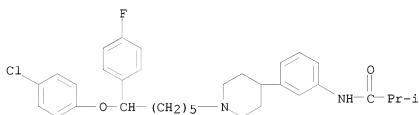
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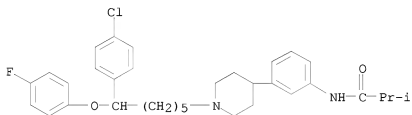
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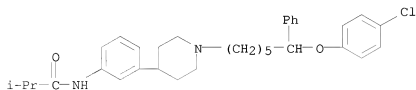
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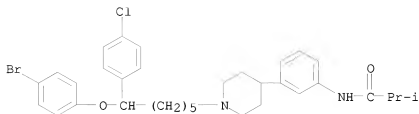
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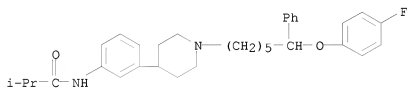
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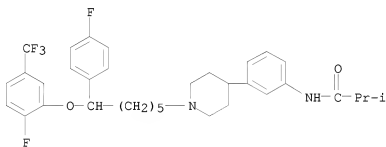
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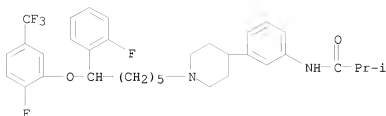
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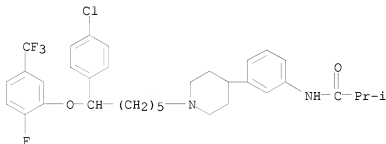
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10/513699



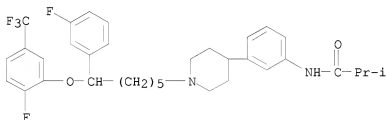
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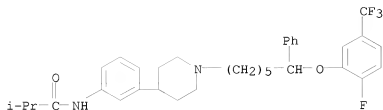
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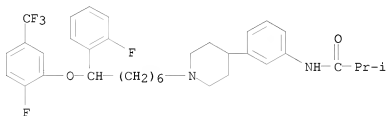
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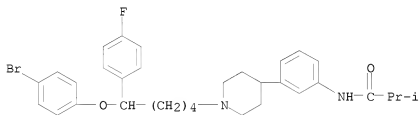
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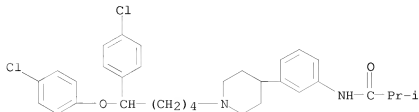
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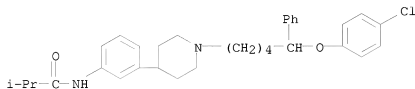
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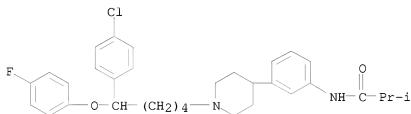
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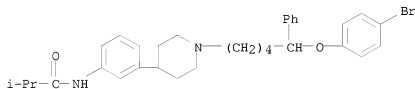
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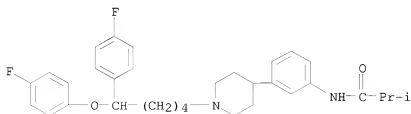
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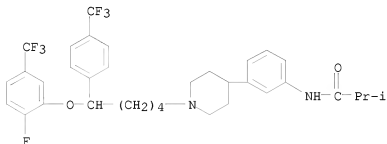
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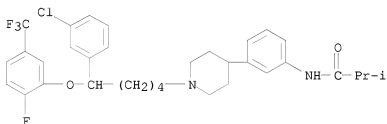
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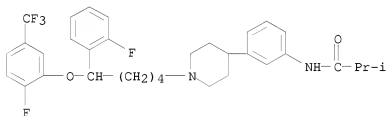
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RN 487057-67-0 CAPLUS

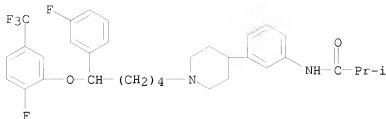
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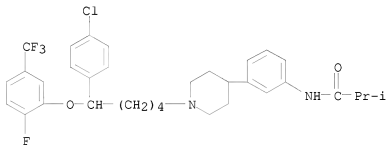
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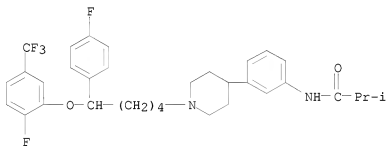
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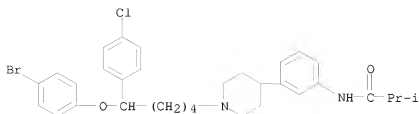


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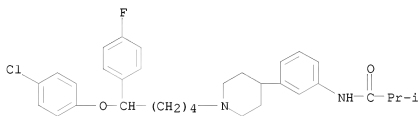


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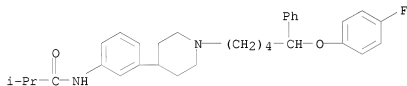
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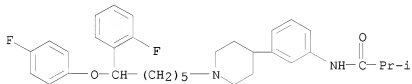
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RN 487057-76-1 CAPLUS
CN Propanamide, N-[3-[1-[5-(4-fluorophenoxy)-5-phenylpentyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)



RN 488098-61-9 CAPLUS
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● HCl

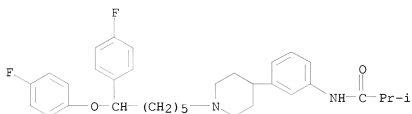
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<12/04/2007>

Erich Leese

10/513699

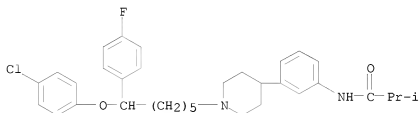
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● HCl

RN 488098-63-1 CAPLUS

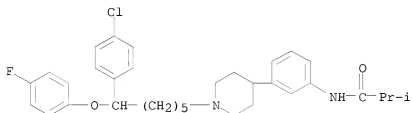
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RN 488098-64-2 CAPLUS

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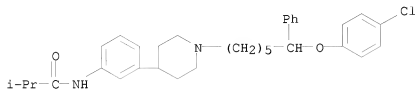


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RN 488098-65-3 CAPLUS

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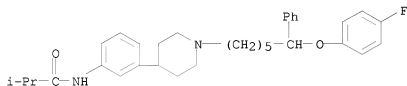
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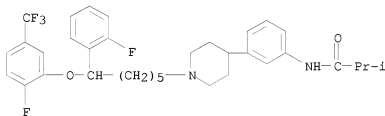
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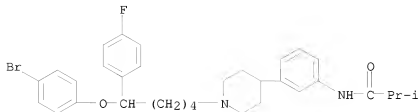
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● HCl

RN 488098-70-0 CAPLUS

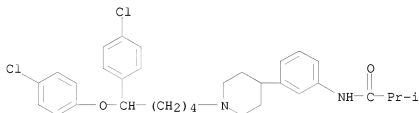
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● HCl

RN 488098-71-1 CAPLUS

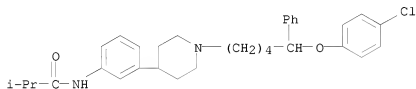
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● HCl

RN 488098-72-2 CAPLUS

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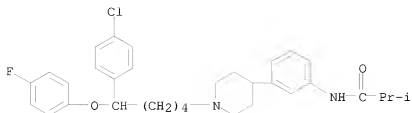


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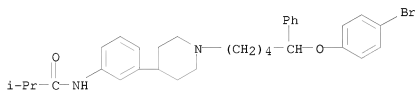
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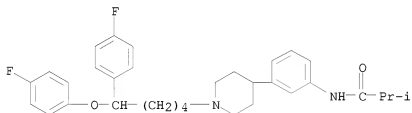
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● HCl

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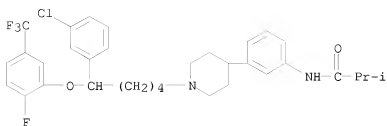


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RN 488098-77-7 CAPLUS

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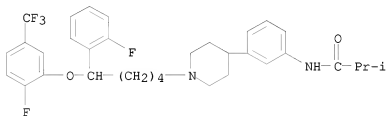
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● HCl

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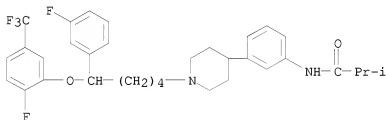
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● HCl

RN 488098-79-9 CAPLUS

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● HCl

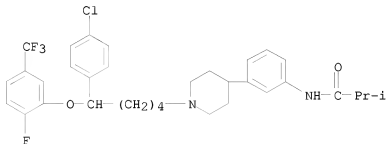
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<12/04/2007>

Erich Leese

10/513699

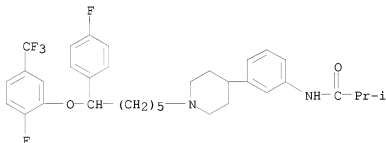
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● HCl

RN 488098-82-4 CAPLUS

CN Propanamide, N-[3-[1-[6-(4-fluorophenyl)-6-[2-fluoro-5-(trifluoromethyl)phenoxy]hexyl]-4-piperidinyl]phenyl]-2-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

REFERENCE COUNT:

3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ACCESSION NUMBER: 2002:31619 CAPLUS

DOCUMENT NUMBER: 136:96697

TITLE: Human melanin concentrating hormone receptor MCH1, its DNA, its synthetic ligands and diagnostic and therapeutic uses thereof

INVENTOR(S): Salon, John A.; Laz, Thomas M.; Nagorny, Raisa; Wilson, Amy E.

PATENT ASSIGNEE(S): Synaptic Pharmaceutical Corporation, USA

PCT Int. Appl., 524 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|---|----------|-----------------|------------|
| WO 2002002744 | A2 | 20020110 | WO 2001-US21350 | 20010705 |
| WO 2002002744 | A3 | 20020808 | | |
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| RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |
| CA 2384358 | A1 | 20020110 | CA 2001-2384358 | 20010705 |
| EP 1246847 | A2 | 20021009 | EP 2001-952456 | 20010705 |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | |
| JP 2004502423 | T | 20040129 | JP 2002-507986 | 20010705 |
| PRIORITY APPLN. INFO.: | | | US 2000-610635 | A 20000705 |
| | | | WO 2001-US21350 | W 20010705 |
| AB | This invention provides an isolated nucleic acid encoding a human MCH1 receptor, a purified human MCH1 receptor, vectors comprising isolated nucleic acid encoding a human MCH1 receptor, cells comprising such vectors, antibodies directed to a human MCH1 receptor, nucleic acid probes useful for detecting nucleic acid encoding human MCH1 receptors, antisense oligonucleotides complementary to unique sequence of nucleic acid encoding human MCH1 receptors, transgenic, nonhuman animals which express DNA encoding a normal or mutant human MCH1 receptor, methods of isolating a human MCH1 receptor, methods of treating an abnormality that is linked to the activity of a human MCH1 receptor, as well as methods of determining binding of compds. to mammalian MCH1 receptors. This invention provides a method of modifying the feeding behavior of a subject which comprises administering to the subject an amount of an MCH1 antagonist effective to decrease the body mass of the subject and/or decrease the consumption of food by the subject. This invention further provides a method of treating a subject suffering from depression and/or anxiety which comprises administering to the subject an amount of an MCH1 antagonist effective to treat the subject's depression and/or anxiety. | | | |
| IT | 387826-65-5P 387826-66-6P 387826-67-7P 387826-68-8P 387826-69-9P 387826-73-5P | | | |

10/513699

387826-74-6P 387826-79-1P 387826-80-4P

387826-81-5P 387826-82-6P 387826-85-9P

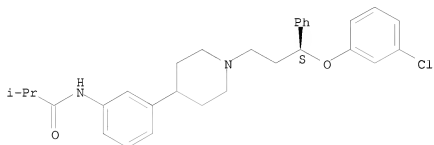
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(human melanin concentrating hormone receptor MCH1, its DNA, its synthetic ligands and diagnostic and therapeutic uses thereof)

RN 387826-65-5 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(3-chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

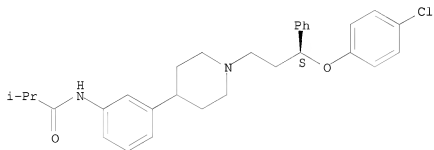
Absolute stereochemistry.



RN 387826-66-6 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(4-chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

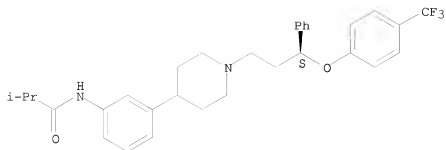
Absolute stereochemistry.



RN 387826-67-7 CAPLUS

CN Propanamide, 2-methyl-N-[3-[1-[(3S)-3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-piperidinyl]phenyl]- (CA INDEX NAME)

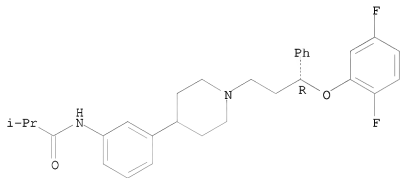
Absolute stereochemistry.



RN 387826-68-8 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-(2,5-difluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

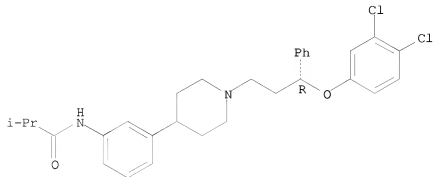
Absolute stereochemistry.



RN 387826-69-9 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-(3,4-dichlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

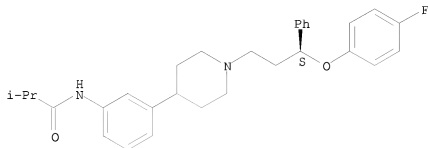


RN 387826-73-5 CAPLUS

10/513699

CN Propanamide, N-[3-[1-[(3S)-3-(4-fluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

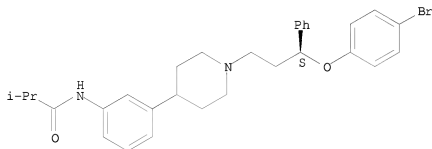
Absolute stereochemistry.



RN 387826-74-6 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(4-bromophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

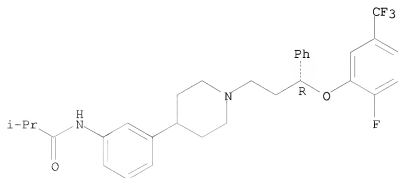
Absolute stereochemistry.



RN 387826-79-1 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-[2-fluoro-5-(trifluoromethyl)phenoxy]-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

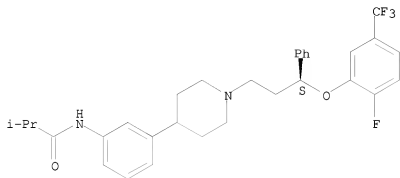


10/513699

RN 387826-80-4 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-[2-fluoro-5-(trifluoromethyl)phenoxy]-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

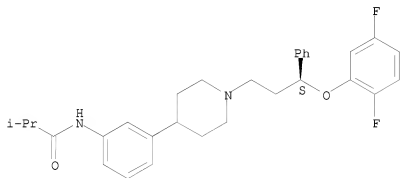
Absolute stereochemistry.



RN 387826-81-5 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(2,5-difluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

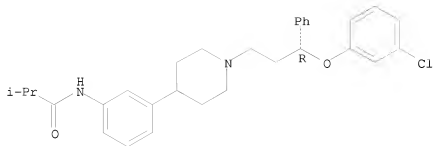


RN 387826-82-6 CAPLUS

CN Propanamide, N-[3-[1-[(3R)-3-(3-chlorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

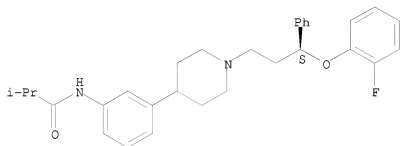
10/513699



RN 387826-85-9 CAPLUS

CN Propanamide, N-[3-[1-[(3S)-3-(2-fluorophenoxy)-3-phenylpropyl]-4-piperidinyl]phenyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

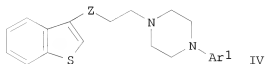
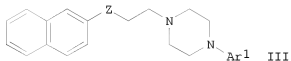
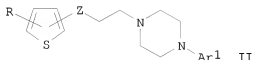
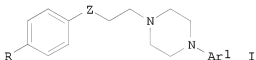


REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2001:76 CAPLUS
 DOCUMENT NUMBER: 134:207795
 TITLE: New 1-aryl-3-(4-arylpiperazin-1-yl)propane derivatives, with dual action at 5-HT1A serotonin receptors and serotonin transporter, as a new class of antidepressants
 AUTHOR(S): Martinez-Esparza, Javier; Oficialdegui, Ana-M.; Perez-Silanes, Silvia; Heras, Begona; Orus, Lara; Palop, Juan-A.; Lasheras, Berta; Roca, Joan; Mourelle, Marisa; Bosch, Ana; Del Castillo, Juan-C.; Tordera, Rosa; Del Rio, Joaquin; Monge, Antonio
 CORPORATE SOURCE: Departments of Medicinal Chemistry and Pharmacology Centro de Investigacion en Farmacobiologia Aplicada (CIFA), Universidad de Navarra, Pamplona, 31080, Spain
 SOURCE: Journal of Medicinal Chemistry (2001), 44(3), 418-428 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:207795
 GI



AB In a search toward new and efficient antidepressants, 1-aryl-3-(4-arylpiperazin-1-yl)propane derivs. I (R = H, Ph, MeO, NO2, Z = CO, CHOH, CHOR1, R1 = 4-F3CC6H4, 4-MeOC6H4, 3,4-OCH3OC6H3, Ar1 =

2-MeOC6H4, 4-ClC6H4, 2-pyridyl, etc.), II (R = H, 2,5-Me2, 5-Me, 5-NO2, Z = CO, CNOH, CHOH, CHOR1, R1 = 4-F3CC6H4, 3,4-OCH2OC6H3, 1-ClOH7, position = 2, 3), III and IV (Ar1 = 2-MeOC6H4, 4-ClC6H4, 2-HOC6H4, Z = CO, CHOH) were designed, synthesized, and evaluated for 5-HT reuptake inhibition and 5-HT1A receptor antagonism. This dual pharmacol. profile should lead, in principle, to a rapid and pronounced enhancement in serotonergic neurotransmission and consequently to a more efficacious treatment of depression. The design was based on coupling structural moieties related to inhibition of serotonin reuptake, such as γ -phenoxypropylamines, to arylpiperazines, typical 5-HT1A ligands. In binding studies, several compds. showed affinity at the 5-HT transporter and 5-HT1A receptors. Antidepressant-like activity was initially assayed in the forced swimming test with those compds. with $K_i < 200$ nM in both binding studies. Functional characterization was performed by measuring the intrinsic effect on rectal temperature in mice and also the antagonism to 8-OH-DPAT-induced hypothermia. The most efficacious compds. II (R = H, Z = CHO-1-ClOH7, position = 3, Ar1 = 2-MeOC6H4) (V), II[R = 5-Me, Z = (E)-CNOH, position = 2, Ar1 = 2-MeOC6H4] and IV (Z = CO, CHOH, Ar1 = 2-MeOC6H4) (VI) were further explored for their ability to antagonize 8-OH-DPAT-induced inhibition of forskolin-stimulated cAMP formation in a cell line expressing the 5-HT1A receptor. Furthermore, the antidepressant-like properties of V and VI, which exhibited 5-HT1A receptor antagonistic property in the latter study, were also evaluated in the learned helplessness test in rats. Among these three compds., VI (Z = CHOH) (1-benzo[b]thiophene-3-yl)-3-[4-(2-methoxyphenyl)-1-ypropan-1-ol] showed the higher affinity at both the 5-HT transporter and 5-HT1A receptors ($K_i = 20$ nM in both cases) and was also active in the other pharmacol. tests. Such a pharmacol. profile could lead to a new class of antidepressants with a dual mechanism of action and a faster onset of action.

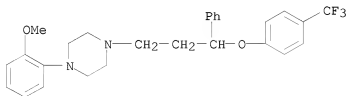
IT 328248-11-9P 328248-15-3P 328248-21-1P
328248-24-4P 328248-26-6P 328248-30-2P
328248-33-5P 328248-36-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation, 5-HT1A serotonin receptor antagonist and serotonin transporter activity, and structure-activity relationship of aryl(arylpiperazinyl)propanes)

RN 328248-11-9 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:2) (CA INDEX NAME)

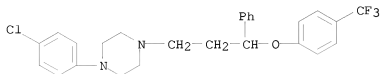


● 2 HCl

10/513699

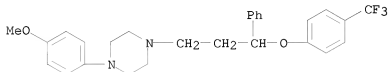
RN 328248-15-3 CAPLUS

CN Piperazine, 1-(4-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



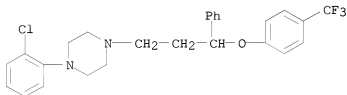
RN 328248-21-1 CAPLUS

CN Piperazine, 1-(4-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



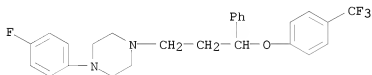
RN 328248-24-4 CAPLUS

CN Piperazine, 1-(2-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 328248-26-6 CAPLUS

CN Piperazine, 1-(4-fluorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:2) (CA INDEX NAME)

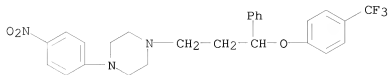


● 2 HCl

RN 328248-30-2 CAPLUS

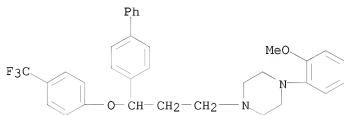
CN Piperazine, 1-(4-nitrophenyl)-4-[3-phenyl-3-[4-

(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 328248-33-5 CAPLUS

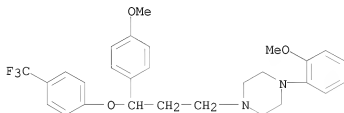
CN Piperazine, 1-([3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)]-, hydrochloride (1:2)
(CA INDEX NAME)



● 2 HCl

RN 328248-36-8 CAPLUS

CN Piperazine, 1-([3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)]-, hydrochloride (1:2)
(CA INDEX NAME)

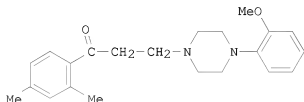


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54

THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

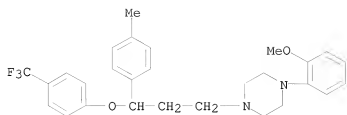
L3 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2000:601312 CAPLUS
 DOCUMENT NUMBER: 133:305272
 TITLE: Design, synthesis and biological evaluation of new 3-[(4-aryl)piperazin-1-yl]-1-arylpropane derivatives as potential antidepressants with a dual mode of action; serotonin reuptake inhibition and 5-HT1A receptor antagonism
 AUTHOR(S): Oficialdegui, A. M.; Martinez, J.; Perez, S.; Heras, B.; Irurzun, M.; Palop, J. A.; Tordera, R.; Lasheras, B.; Del Rio, J.; Monge, A.
 CORPORATE SOURCE: Department of Medicinal Chemistry, Centro de Investigacion en Farmacobiologia Aplicada (CIFA), Universidad de Navarra, Pamplona, 31080, Spain
 SOURCE: Farmaco (2000), 55(5), 345-353
 CODEN: FRMCE8; ISSN: 0014-827X
 PUBLISHER: Elsevier Science S.A.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 133:305272
 GI



I

- AB It has been suggested that the combination of a selective serotonin reuptake inhibitor (SSRI) and a 5-HT1A receptor antagonist may facilitate the onset of the SSRIs antidepressant action. Accordingly, we describe the synthesis of a series of new 3-[(4-aryl)piperazin-1-yl]-1-arylpropane derivs. with structural modifications performed in Ar1, Ar2 and Z (Z is different functional groups) to obtain the sought dual activity. Comps. were evaluated for in vitro affinity at 5-HT1A receptors and 5-HT transporter. The antidepressant-like activity of derivs. with the higher affinity was assessed initially using the forced swimming test (FST). Compound 1-(2,4-dimethylphenyl)-3-[(2-methoxyphenyl)piperazin-1-yl]-1-propanone (I) showed the best antidepressant-like activity which was further confirmed in the learned helplessness test.
- IT 302561-62-2P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (design, synthesis and antidepressant activity of [(aryl)piperazinyl]arylpropane derivs.)
- RN 302561-62-2 CAPLUS
- CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methylphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

10/513699



REFERENCE COUNT:

42

THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:655827 CAPLUS

DOCUMENT NUMBER: 121:255827

ORIGINAL REFERENCE NO.: 121:46707a, 46710a

TITLE: Preparation of (hetero)arylpropanolamine derivatives as cerebral calcium overload blockers

INVENTOR(S): Jakobsen, Palle; Kanstrup, Anders; Lundbeck, Jane Marie

PATENT ASSIGNEE(S): Novo Nordisk A/S, Den.
SOURCE: Eur. Pat. Appl., 18 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|----------|
| EP 576766 | A1 | 19940105 | EP 1992-610053 | 19920629 |

R: GB

PRIORITY APPLN. INFO.: EP 1992-610053 19920629

OTHER SOURCE(S): MARPAT 121:255827

AB XR3(RO)CCR4R5CR6R7NR1R2 [X = Ph optionally substituted with one or more cyano, halo, haloalkyl, alkoxy, alkyl, alkanoyl, alkenyl, aryloxy, aralkoxy, amino, alkyl mono or disubstituted amino, alkanoylamino, carbamoyl, alkyl mono- or disubstituted carbamoyl, alkyl substituted with amino, alkyl mono or disubstituted amino, NO₂, morpholino, imidazolyl; R = 3,4-methylenedioxyphenyl, aryl or heteroaryl all of which can be optionally substituted with one or more cyano, halogeno, alkyl, alkoxy, alkenyl, trifluoromethyl, alkylene, aryloxy, aralkoxy, alkylthio; R₁, R₂ = alkyl, cycloalkyl, alkenyl, cycloalkylalkyl, all of which can be unsubstituted or substituted with alkyl, alkoxy or cyano; R₁R₂ = 5-, 6- or 7-membered ring containing ≥1 N atom, or which optionally contains 2 N atoms, one or 2 O atom(s) or one or 2 S atom(s) or a combination thereof, which ring is optionally substituted with alkyl, alkoxy, or aryl; and R₃-R₇ = H, alkyl, phenyl; R₄X = carbocyclic ring containing 5 or 6 atoms; or salts thereof with a pharmaceutically acceptable acid; with provisos], were prepared. Thus, 1-(4-cyanophenyl)-3-piperidinylpropan-1-ol was condensed with 4-trifluoromethylbenzotrifluoride using KOCMe₃ to give 1-[3-(4-cyanophenyl)-3-(4-trifluoromethylphenoxy)propyl]piperidine, isolated as the oxalate. The latter inhibited stimulated uptake of ⁴⁵Ca by rat P2 synaptosomal preps. with IC₅₀ = 2.2 µg/mL, vs. 26 µg/mL for nifedipine. Generic I formulations are given.

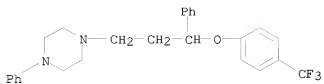
IT 158545-85-8P 158546-06-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as cerebral calcium overload blocker)

RN 158545-85-8 CAPLUS

CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-
(CA INDEX NAME)

10/513699



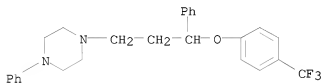
RN 158546-06-6 CAPLUS

CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 158545-85-8

CMF C26 H27 F3 N2 O



CM 2

CRN 144-62-7

CMF C2 H2 O4



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 'HS' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS ----- GI and AB
 ALL ----- BIB, AB, IND, RE
 APPS ----- AI, PRAI
 BIB ----- AN, plus Bibliographic Data and PI table (default)
 CAN ----- List of CA abstract numbers without answer numbers
 CBIB ----- AN, plus Compressed Bibliographic Data
 CLASS ----- IPC, NCL, ECLA, FTERM
 DALL ----- ALL, delimited (end of each field identified)
 DMAX ----- MAX, delimited for post-processing
 FAM ----- AN, PI and PRAI in table, plus Patent Family data
 FBIB ----- AN, BIB, plus Patent FAM
 IND ----- Indexing data
 IPC ----- International Patent Classifications
 MAX ----- ALL, plus Patent FAM, RE
 PATS ----- PI, SO
 SAM ----- CC, SX, TI, ST, IT
 SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
 SCAN must be entered on the same line as the DISPLAY,
 e.g., D SCAN or DISPLAY SCAN)
 STD ----- BIB, CLASS

 IABS ----- ABS, indented with text labels
 IALL ----- ALL, indented with text labels
 IBIB ----- BIB, indented with text labels
 IMAX ----- MAX, indented with text labels
 ISTD ----- STD, indented with text labels

 OBIB ----- AN, plus Bibliographic Data (original)
 OIBIB ----- OBIB, indented with text labels

 SBIB ----- BIB, no citations
 SIBIB ----- IBIB, no citations

 HIT ----- Fields containing hit terms
 HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
 containing hit terms
 HITRN ----- HIT RN and its text modification
 HITSTR ----- HIT RN, its text modification, its CA index name, and
 its structure diagram
 HITSEQ ----- HIT RN, its text modification, its CA index name, its
 structure diagram, plus NTE and SEQ fields
 FHITSTR ----- First HIT RN, its text modification, its CA index name, and
 its structure diagram
 FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
 structure diagram, plus NTE and SEQ fields
 KWIC ----- Hit term plus 20 words on either side
 OCC ----- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the

10/513699

information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.

ENTER DISPLAY FORMAT (BIB):.

10/513699

L3 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
AN 2009:412461 CAPLUS
DN 151:496
TI QSAR study of the 5-HT1A receptor affinities of arylpiperazines using a
genetic algorithm-artificial neural network model
AU Habibi-Yangjeh, Aziz
CS Department of Chemistry, Faculty of Science, University of Mohaghegh
Ardabili, Ardabil, Iran
SO Monatshefte fuer Chemie (2009), 140(5), 523-530
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DT Journal
LA English
RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE 'REGISTRY' ENTERED AT 18:23:49 ON 29 JUN 2009

L1 STRUCTURE UPLOADED

L2 211 S L1 FULL

FILE 'CAPLUS' ENTERED AT 18:24:36 ON 29 JUN 2009

L3 17 S L2 FULL

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

98.13

284.23

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

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